A Probabilistic Model and Process to Assess Risks to Aquatic Organisms

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Executive Summary

Background

The U.S. EPA is implementing a new tiered process for conducting ecological risk assessment, which will be used under the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) regulatory framework. This process is being carried out by the Environmental Fate and Effects Division (EFED) of the Office of Pesticide Programs. This approach will include the use of probabilistic tools at the more refined levels (tiers) of the risk assessment process. The aim of this process is to provide information on the probability or likelihood of ecological impact, and on the magnitude or severity of the effect. The results of probabilistic analyses will be used by risk managers in their decision-making process.

In 1996, the Agency's Scientific Advisory Panel (SAP) endorsed the risk quotient approach as a suitable screening method to identify pesticide uses of potential concern that warrant refined assessment. The SAP suggested that EFED incorporate probabilistic methods into such refined assessments, noting that such approaches can provide estimates of the probability and magnitude of effects.

Over the past three years, EFED, along with individuals from academia, industry, and non-governmental organizations, has worked to develop a suite of refined risk assessment methods through the Ecological Committee on FIFRA Risk Assessment Methods (ECOFRAM) initiative. Concluded in 1999, reports originating out of the ECOFRAM initiative served as the basis for development of an EFED implementation plan for conducting probabilistic ecological risk assessments. This implementation plan, presented to the SAP in April of 2000, outlined a proposed general approach for assessing pesticide risks to birds and aquatic organisms, including the use of probabilistic tools in a tiered manner.

As part of the process of developing and implementing a probabilistic approach for ecological risk assessment, EFED has completed a case study. The case study involved both deterministic and probabilistic risk assessments for ChemX.

In the deterministic, screening-level assessment, risks to birds and aquatic organisms from exposure to ChemX were concluded to be high. It was determined that a refinement of the risk assessment was warranted. The refined risk assessment presented herein follows the approaches outlined in EFED's implementation plan for conducting probabilistic terrestrial and aquatic organism risk assessments. The case study is designed to express risk in more quantitative terms than in the deterministic approach, to better understand the likelihood and magnitude of expected effects to fish and aquatic invertebrates.

For this case study, the aquatic assessment was limited to 4 crops for a single chemical example and product formulation. Specific usage characteristics were considered important in deciding which crops to examine: (1) application rate, (2) associated estimated exposure concentrations, (3) acreage treated, and (4) representativeness of the use site. Corn, cotton, potatoes, and grapes were the use scenarios selected for the case study analysis. The variety of crops, regions, use rates, and scenarios selected represent a broad and reasonably comprehensive selection for uses of a chemical.

For each acute effects assessment for a given species, a distribution of estimated exposure and a distribution of toxicity were combined in a joint probability function through Monte Carlo analysis. The resultant function allows the expression of risk in terms of the likelihood, or probability, of an exposure concentration occurring, and the related magnitude of effect in percent mortality within a given species expected to occur at that level. For each chronic assessment, a distribution of exposure concentrations was compared to a chronic effect point estimate. The chronic analyses give information only on the probability that the chronic endpoint assessed would be exceeded, not on the magnitude of chronic effect expected. In both acute and chronic assessments, estimated environmental concentrations generated from PRZM/EXAMS simulation modeling were directly compared to the toxic effect in the laboratory at the same exposure concentration (i.e., internal dose to the animal was not considered).

A deterministic screen conducted on ChemX concluded qualitatively that it can pose a high risk to aquatic organisms. Through the deterministic risk quotient method, the acute restricted use Level of Concern (LOC) was exceeded for freshwater fish for all crops examined. For freshwater invertebrates, the acute high risk LOC was exceeded for most of the crops examined. The chronic LOC was exceeded for fish for potatoes, sorghum , and grapes, in a comparison of the peak estimated environmental concentrations to chronic no-observed-effects-concentration, while chronic the LOC was exceeded for all crops for freshwater invertebrates. Based on the probabilistic analysis undertaken herein, it was concluded that the use of ChemX was expected to infrequently (5% of the time or less) result in significant freshwater fish mortalities, but routinely result in reduced growth and other chronic effects in exposed fish. Substantial mortalities and chronic effects to sensitive aquatic invertebrates were predicted to routinely occur after peak exposures. It was concluded that estuarine fish and invertebrates, which are more sensitive than their freshwater relatives, are likely to experience substantial mortality when exposed to concentrations in their habitat equivalent to what has been modeled for farm ponds in the use scenarios studied.

The probability of high mortality rates for invertebrates would be likely to have an indirect effect on fish, as would the high probability of exceeding invertebrate chronic no-effects concentrations. Indirect effects on fish could include reduced juvenile fish survival due to reduced invertebrate food resources, with concomitant potential alterations in fish population structure, and potential decreases in fish populations or other higher trophic levels.

Sublethal effects on fish from acute exposures to ChemX were not addressed. These endpoints are generally not assessed by the standard toxicity test protocols used by EFED, but sublethal effects from acute exposure should be considered, at least qualitatively, when evaluating the risk to fish from a chemical. Were dose-response data for acute effects of ChemX available, these data could have been used in the probabilistic model developed.

There are a number of uncertainties associated with both the refined and deterministic risk assessments that are not included in this case study risk assessment. These include uncertainty regarding the error introduced when extrapolating from laboratory to field effects. For example, mortality in the field could be greater in populations previously stressed by other pesticide exposures, habitat loss, predation, temperature stress, or competition for limited resources, among other things. Overall field mortality could be lower if the laboratory population were to represent an unusually sensitive species. There is uncertainty associated with the use of single laboratory toxicity tests for a species. The experimental uncertainty regarding the representativeness of the test results could be reduced through replication of the toxicity tests for each species. There is uncertainty regarding the extrapolation of expected effects to more sensitive species, and the frequency with which these more sensitive species occur in ChemX use areas. There is uncertainty regarding the extrapolation to all invertebrates from a data set containing only arthropods. There is also uncertainty regarding the representativeness of the fate input parameters used in the exposure modeling; some input parameters were based on limited physico-chemical data. Another source of uncertainty is the use of exposure model-derived estimated concentrations to represent actual environmental concentrations. These uncertainties could , in general, be reduced through additional field testing and measurement.

The uncertainties that were addressed in the probabilistic analyses, and which are included in the confidence bounds given for the risk estimates, reflect uncertainty in the risk analysis construct and primarily regard the fits of the applied distributions to the data. The risk analysis construct for this assessment involved the use of PRZM/EXAMS model exposure data and laboratory toxicity data as fit by a log-probit model. As noted above these uncertainty estimates reflect only a portion of the true uncertainty. However, the uncertainty expressed does address the fact that there is uncertainty in the estimates of risks indicated by the RQs, and is an effort to provide quantitative estimates of detrimental effect and bounds on those effect estimates.

The ChemX incident history for fish is relatively scant in comparison to birds, and the probabilistic analysis explains that large die-offs would be an infrequent, though real, occurrence. Invertebrates can be expected to suffer more routine mortalities and other ill effects, although these would be unlikely to be captured in an incident report due to their subtlety. Similarly, sublethal and chronic effects to fishes would not be tractable through incident reports. Nevertheless, use of ChemX would be expected to pose real and significant risks, acutely and chronically, to aquatic organisms.

I. Introduction

A deterministic risk assessment was conducted for flowable ChemX uses. This deterministic assessment addressed risks to aquatic organisms through the application of the EFED risk quotient method. EFED also typically analyzes available wildlife effects field studies, monitoring programs, publically available literature, and reports of incidents of adverse effects on aquatic and terrestrial organisms associated with field uses. The risk quotient assessment and field study/incident analysis lead EFED to conclude that the risks to birds and other wildlife by ChemX is extremely high. The deterministic assessment concluded that the weight of evidence for effects on birds was extensive, leading to a high level of certainty in concluding high risks to these organisms. The deterministic assessment also concluded that ChemX poses a high risk to fish and aquatic invertebrates.

It was clear from the results of the ChemX deterministic screen that refinement of the risk assessment was warranted. This case study presents a refined risk assessment for selected ChemX uses. The refined risk assessment presented follows the approaches outlined in EFED's implementation plan for conducting probabilistic terrestrial and aquatic organism risk assessments. This chapter focuses on aquatic risks and contains the following elements:

- Problem Formulation: This section (1) reviews the current status of ChemX registrations, (2) presents the results of a ChemX screening assessment, (3) discusses the extent of each use registration, (4) presents the application scenarios selected for risk assessment, (5) describes the selection process for these scenarios and the species used for analysis, and (6) discusses the measurement and asessment endpoints selected for the risk assessment

- Risk Assessment Model: This section (1) provides a general overview of the risk assessment model, (2) presents a detailed description of the exposure model, including assumptions used and parameterization of model variables, (3) discusses the effects model and parameterization of applicable variables, and (4) describes the methods for integrating the exposure and effects models for risk assessment output

- Model Scenario Matrix: This section describes the full extent of combinations of crop, pesticide application method, application rate, exposure model options, and effects variables and assumptions that are addressed in the risk assessment

- Results: This section presents the results of application of the risk assessment model

- Sensitivity Analysis: This section describes the parameters used in the assessment, how they were varied, and what was their influence on model output.

- Discussion: This section presents a review and discussion of major results and conclusions.

- Risk Characterization: This section provides interpretation of these results and characterizes risks.

II. Problem Formulation

There are many use scenarios in a mature registration such as ChemX and therefore many permutations of risk which could be considered. Resources to consider all of these in a probabilistic refinement would be prohibitively exhaustive and unnecessary. Therefore, this case study addresses only a select few scenarios chosen for their representativeness of the many use patterns, and includes those with the greatest proportion of use and/or which may pose the greatest risk to aquatic organisms

A . Review of ChemX Registrations and Uses

ChemX is a pesticide. It is used in several formulations for a wide variety of crops. Currently between 1 and 3 million pounds of ChemX are used annually on 2 to 4 million acres in the United States. Presently, most of it is used on alfalfa, field corn, grapes, potatoes, sorghum, tobacco, sunflower, soybeans, and cotton.

To further discriminate among the uses of greatest concern, EFED consulted the Biologic and Economic Analysis Division's application overview report of ChemX uses. Corn, alfalfa, and cotton uses account for the greatest acres currently treated. In recent years, approximately 2 million acres of corn were treated, easily ranking as the largest crop use, although representing a low percent of the total corn acreage. The volume of Chem X used on this crop totaled approximately 2 million pounds of active ingredient. At another extreme, applications to grapes appear to be confined to several counties, comprising only about 25,000 acres treated annually but with the highest use rate, approximately 3 times the corn use rate. Potatoes fall between the extreme but have the highest proportion of its acreage treated (>10%). Due to its relatively large acreage treated (up to 700 thousand acres) and its association with freshwater ponds, cotton is another crop of interest

B. Review of Deterministic Screening Results for Flowable Uses

In order to support the goal of the refined risk assessment efforts to focus on those uses of ChemX found to pose the highest risk, EFED first reviewed the risk quotients calculated for each set of application scenarios modeled in the deterministic risk assessment. As stated in the introduction, the deterministic screen concluded that the risks of flowable ChemX to fish and aquatic invertebrates were high. The following table present the ranges of acute and chronic risk quotients associated with each general crop type. In order to provide an estimate of the chronic no-effect concentration for the most sensitive species tested in acute tests, bluegill, the acute-to-chronic ratio for a tested, though less sensitive, species was applied to the bluegill acute data. The bluegill Estimated No-Effect Concentration (ENEC) was thus calculated by dividing the bluegill LC_{50} by the acute-to-chronic ratio derived for rainbow trout.

Table 1. Risk Quotients for Freshwater Fish Based on Bluegill Sunfish LC50 value of 0.088 ppm, a Rainbow Trout ELS NOEC of 24.8 ppb and a Bluegill Sunfish ENEC (Estimated No-Effect Concentration) of 5.72 ppb .

Crop site Rate in lbs ai/acre (No. of applications)	LC_{50}[1] (ppm)	NOEC[2] (ppm)	ENEC[3] (ppm)	Peak EEC[4] (ppm)	Acute RQ (Peak EEC/ LC50)	Chronic RQ (Peak EEC/ NOEC)	Chronic RQ (Peak EEC/ ENEC)
Potatoes 1.0 (3)	0.088	0.0248	0.00572	0.0274	0.31*	1.10***	4.80***
Cotton 1.0 (1)	0.088	0.0248	0.00572	0.0133	0.15*	0.54	2.33***
Grapes 10 (1)	0.088	0.0248	0.00572	0.0394	0.45*	1.59***	6.89***
Corn 1.0 (2)	0.088	0.0248	0.00572	0.0151	0.17*	0.61	2.64***
Alfalfa 1.0 (1)	0.088	0.0248	0.00572	0.0130	0.15*	0.52	2.27***
Sorghum 1.3 (2)	0.088	0.0248	0.00572	0.0307	0.35*	1.24***	5.37***

* RQ exceeds the endangered species and restricted use LOC
** RQ exceeds the high concern for acute risk LOC
*** RQ exceeds the chronic risk LOC
[1] LC_{50}: Concentration predicted to result in 50% mortality in the laboratory
[2] NOEC: No-Observed-Effect-Concentration for laboratory chronic toxicity test
[3] ENEC: Estimated No-Observed -Effect-Concentration (see text above for explanation)
[5] EEC: Estimated Environmental Concentration based on exposure simulation model PRZM/EXAMS

Table 2. Risk Quotients for Freshwater Invertebrates Based on a *Daphnia magna* LC50 value of 0.029 ppm and a NOEC of 0.0098 ppm.

Crop Site	Rate in lbs ai/A (No. of Appl.)	LC50 (ppm)	NOEC (ppm)	EEC Peak (ppm)	Acute RQ (Peak EEC/ LC50)	Chronic RQ (Peak EEC/ NOEC)
Potatoes	1.0 (3)	0.029	0.0098	0.0274	0.95 **	2.80 ***
Cotton	1.0 (1)	0.029	0.0098	0.0133	0.46*	1.38***
Grapes	10 (1)	0.029	0.0098	0.0394	1.36**	4.02***
Corn	1.0 (2)	0.029	0.0098	0.0151	0.52**	1.54***
Alfalfa	1.0 (1)	0.029	0.0098	0.0130	0.45*	1.33***
Sorghum	1.3 (2)	0.029	0.0098	0.0307	1.06**	3.13***

* RQ exceeds the endangered species and restricted use LOC's
** RQ exceeds the high concern for acute risk LOC
*** RQ exceeds the chronic risk LOC

Table 3. Risk Quotients for Estuarine/Marine Fish Based on an Atlantic Silverside LC50 value of 0.033 ppm and a Sheepshead minnow NOEC of 0.0026 ppm.

Crop site	Rate in lbs ai/A (No. of Apps.)	LC50 (ppm)	NOEC (ppm)	EEC Peak (ppm)	Acute RQ (Peak EEC /LC50)	Chronic RQ (Initial EEC/ NOEC)
Potatoes	1.0 (3)	0.033	0.0026	0.0274	0.83**	10.54***
Cotton	1.0 (1)	0.033	0.0026	0.0133	0.40*	5.12***
Grapes	10 (1)	0.033	0.0026	0.0394	1.19**	15.15***
Corn	1.0 (2)	0.033	0.0026	0.0151	0.46*	5.81***
Alfalfa	1.0 (1)	0.033	0.0026	0.0130	0.39*	5.00***
Sorghum	1.3 (2)	0.033	0.0026	0.0307	0.93**	11.81***

* RQ exceeds the endangered species and restricted use LOC's
** RQ exceeds the high concern for acute risk LOC
*** RQ exceeds the chronic risk LOC

Table 4. Risk Quotients for Estuarine/Marine Invertebrates Based on a Pink Shrimp LC50 value of 0.0046 ppm and a Mysid shrimp NOEC of 0.0004 ppm.

Crop site	Rate in lbs ai/A (No. of Apps.)	LC50 (ppm)	NOEC (ppm)	EEC Peak (ppm)	Acute RQ (Peak EEC /LC50)	Chronic RQ (Initial EEC/ NOEC)
Potatoes	1.0 (3)	0.0046	0.0004	0.0274	5.96**	68.50***
Cotton	1.0 (1)	0.0046	0.0004	0.0133	2.89**	33.25***
Grapes	10 (1)	0.0046	0.0004	0.0394	8.57**	98.50***
Corn	1.0 (2)	0.0046	0.0004	0.0151	3.28**	37.75***
Alfalfa	1.0 (1)	0.0046	0.0004	0.0130	2.85**	32.50***
Sorghum	1.3 (2)	0.0046	0.0004	0.0307	6.67**	76.75***

* RQ exceeds the endangered species and restricted use LOC's
** RQ exceeds the high concern for acute risk LOC
*** RQ exceeds the chronic risk LOC

Freshwater fish acute RQ values exceeded the acute restricted use risk LOC of 0.1 for use on potatoes, sorghum and grapes, and range from 0.31 to 0.45. The cotton, corn, and alfalfa use acute RQs were slightly less but still exceed the acute restricted use risk LOC, at 0.15 to 0.17. Freshwater fish chronic RQ values based on a comparison of peak EEC to rainbow trout NOEC, exceeded the chronic LOC for potatoes, sorghum and grapes, and range from 1.1 to 1.59. However, based on a comparison of peak EEC to *bluegill* ENEC, freshwater fish chronic RQ values all exceed the chronic LOC. For freshwater invertebrates, high risk use LOC was nearly met or exceeded, with RQs ranging from 0.45 to 1.36, with potatoes, sorghum, and grapes still giving the highest values. ChemX usage on all crops yielded exceedences of the chronic LOC for freshwater invertebrates.

Risk for estuarine/marine fish and invertebrates was higher for all crops, with acute RQs frequently exceeding the acute high risk LOC, and all values exceeding the chronic risk LOC, when comparing peak EEC to NOEC.

In summary, risk of mortality is predicted for freshwater fish under some conditions. Chronic adverse effects are indicated for freshwater fish for some crops, based on a comparison of chronic endpoints with peak exposures. The risk of mortality was greater for invertebrates, and was highest for the same three crops posing the highest risk to fish (potatoes, sorghum, grapes). Chronic effects on invertebrates are predicted for all crops modeled, based on a peak exposure/ chronic endpoint comparison. Due to their greater sensitivity to ChemX, risk to estuarine species are predicted to be higher than that of freshwater species, if exposure concentrations in estuarine environments attain the same level as that estimated for the farm pond scenario.

C. Use Scenarios Selected for Probabilistic Assessment

Scenarios were selected on the basis of (1) acreage treated, (2) risk quotients, (3) application rates, and (4) representativeness of the use site. The selected scenarios for the aquatic risk assessment were corn, cotton, potatoes, and grapes.

The following table provides an analysis of ChemX usage on various major acreage crops (25K or more acres treated) from 1990-1996, and risk estimates associated with these uses. Acres of crop treated were evaluated, along with acute and chronic risk RQs. Based on these data, the usage and risk data fall into three classes for aquatic organisms: (1) High use crops with relatively low RQs, (2) Intermediate use crops with intermediate RQs, (3) Low use crops with high RQs.

Corn, alfalfa, and cotton fell into the first class with use ranging from 300,000 to 1,500,000 acres treated per year, and RQs for these crops falling into similar classes. For example, freshwater fish acute RQs for these crops were all in the range of 0.2 and chronic RQs in the range of 2.5, based on the bluegill ENEC. Freshwater invertebrate acute RQs were in the range of 0.5, and chronic RQs in the range of 1.5. Based on comparison with other uses, these RQs were given a relative ranking of third out of three for all species. That is, the relative risk was lowest among three classes of crops.

Potatoes and sorghum fell into the intermediate classification, with use approximately 200,000 acres/year. RQs were greater than for corn, cotton and alfalfa, but less than for grapes. Freshwater fish acute RQs for potatoes and sorghum were in the range of 0.3, and chronic RQs, based on the bluegill ENEC, were in the range of 5. Freshwater invertebrate acute RQs were in the range of 1, and chronic RQs in the range of 3. Based on comparison with other uses, these RQs were given a relative ranking of second out of three for all species.

Grapes, sunflower, winter wheat, soybeans and hay fell into the lowest use classification, with less than 70,000 acres treated with ChemX per year. There were no deterministic RQs generated in the deterministic screen for sunflower, winter wheat, soybeans and hay. Of the crops assessed, grapes yielded the highest RQs, with freshwater fish acute RQs for grapes of 0.45 and chronic RQs in the range of 7. Freshwater invertebrate acute RQs were in the range of 1.5, and chronic RQs in the range of 4.

Table 5. Analysis of ChemX Usage 1990-1996 From Use Data and Associated Aquatic Risk Quotients[1]. Major Acreage uses (Crops with 25K acres or more treated).

Crop	Acres Treated (Thousands of acres, Wtd Ave)	Major States for Usage	RQs Fish: Freshwater Acute,Chronic ___________ Saltwater Acute, Chronic	Relative Ranking of RQs for Fish	RQs Invertbrates: Freshwater Acute,Chronic ___________ Saltwater Acute, Chronic	Relative Ranking of RQs for Invertebrates
Corn RQs based on OH	1500	NE, IL, KS, IA, IN, TX	0.17, 2.64	3	0.52, 1.54	3
			0.46, 5.81	3	3.28, 37.75	3
Alfalfa RQs based on CA	800	CA, OK, KS, CO, UT, KY	0.15, 2.27	3	0.45, 1.33	3
			0.39, 5.00	3	2.85, 32.50	3
Cotton RQs based on MS	300	TX, OK, MS, AR	0.15, 2.33	3	0.46, 1.38	3
			0.40, 5.12	3	2.89, 33.25	3
Sorghum RQs based on TX	200	KS, TX, NE, FL, MO	0.35, 5.37	2	1.06, 3.13	2
			0.93, 11.81	2	6.67, 76.75	2
Potatoes RQs based on ME	200	ND, ID, FL, MN, WA, WI	0.31, 4.80	2	0.95, 2.80	2
			0.83, 10.54	2	5.96, 68.50	2
Sun-flower	70	ND, KS, SD	NC[2]	NC[2]	NC[2]	NC[2]
Winter Wheat	50	LA, OK, TX, CO, KY, KS	NC[2]	NC[2]	NC[2]	NC[2]
Soybean	40	DE, NC, KY, IL, VA, ND	NC[2]	NC[2]	NC[2]	NC[2]
Hay, Other	30	PA, MT, IA, MD, IL, CA	NC[2]	NC[2]	NC[2]	NC[2]
Grapes RQs based on CA	25	CA	0.45, 6.89	1	1.36, 4.02	1
			1.19, 15.15	1	8.57, 98.50	1

[1]RQs do **NOT** take into account PCAs, all PRZM/ EXAMS EECs based on 100% cropped area, 100% crop treated. EECs based on usage of flowable product. Chronic RQs use intial EEC**.**
[2]NC indicates not calculated in original deterministic risk assessment.

Based on this analysis, it was decided that a probabilistic analysis would be conducted on representative crops from each use/risk classification. Therefore, corn and cotton were selected to represent high use, low RQ crops. Potatoes were selected to represent intermediate use, intermediate RQ crops. Grapes were selected to represent low use, high RQ crops.

Regional aspects of ChemX use also served to focus the risk assessment use scenarios to certain areas within the United States. Based on the high use of ChemX in midwest corn, scenarios in Iowa and Ohio were chosen. The Yazoo basin in Mississippi was selected for cotton, as were scenarios in Maine and Florida for potatoes and California for grapes. The variety of crops, regions, use rates, and scenarios represent a broad and reasonably comprehensive selection for flowable uses of ChemX.

D. Assessment and Measurement Endpoints

Assessment endpoints are Aexplicit expressions of the actual environmental value that is to be protected@ (USEPA 1992). For this risk assessment, which deals with a variety of pesticide use sites and variable environmental settings, the assessment endpoint is by necessity generic. Using the results of the deterministic risk assessment, the aquatic assessment will focus on the prediction of the probability and magnitude of acute mortality to fish and aquatic invertebrates and a consideration of population/community consequences. Sensitive life stage and likely chronic effects are also examined.

The measurement endpoints upon which the assessment is constructed include acute lethality and chronic endpoint testing with ChemX technical in aquatic organisms under laboratory conditions of exposure and observation. Chronic measurement endpoints included survival and growth in fish, and survival, growth, and reproductive success (young/adult/reproduction day) in invertebrates.

Probabilistic estimations of risk are presented for expectations of acute mortality. Exceedence frequency analyses were conducted for freshwater species chronic assessments, in the form of estimates of the frequency of exceeding chronic effect point estimates.

E. Aquatic Organism Risk Assessment Considerations

1. Focal Species Selection

a. Fish

Generic fish species representing species with a 5^{th} percentile (most sensitive), 50^{th} percentile (or median), and a 95^{th} percentile sensitivity (least sensitive) to ChemX were analyzed to advance the assessment beyond consideration of just the standard freshwater test species (bluegill sunfish and rainbow trout). It is assumed that the distributions of sensitivity represent the range of responses that are likely to be encountered in the environment.

Acceptable acute toxicity data for ChemX were available on 8 species of freshwater fish in 5 families and 1 species of saltwater fish (Mayer and Ellersieck, 1985; USEPA, 1986). Multiple tests were available for the rainbow trout, brown trout, fathead minnow, bluegill and the yellow perch. For these species with multiple tests, a geometric mean of the estimated LC50s, within a given species was used in tabulating a distribution of toxicity. In developing a sensitivity curve for freshwater fish with the available data, species’ data were combined into their respective families. This was done because all families except salmonids had a single representative species, whereas, salmonids had four representatives. The aim was not to skew the sensitivity data by over-representation with salmonids. The geometric mean of the multiple species and/or multiple tests with the same species was used in establishing points along the species sensitivity curve.

Mayer and Ellersieck utilized the graphical Litchfield-Wilcoxon method (Litchfield and Wilcoxon, 1949) for estimating the LC50 which does not provide an estimate of the standard error for the dose-response curve. For this reason the original data from the Columbia National Fish Laboratory were obtained (courtesy Denny Buckler) and a SAS probit method (SAS version 6.12, 1996) was employed to recalculate the LC50s. The following table provides the recalculated data which differ slightly from the data reported in the deterministic screen.

Table 6. ChemX Recalculated Fish Toxicity (SAS Probit)

Species	LC_{50} (ppb)	Slope
Rainbow trout	306	3.2
Steelhead	606	4.2
Brown trout	578	8.8
Brown trout	280	- -
geomean brown trout	402	- -
Coho salmon	486	8.3
Lake trout	140	- -
geomean salmonids	356	mean salmonids 6.1
Bluegill	104	6.8
Yellow perch	110	3.7
Yellow perch geo mean perch	358 198	4.0 mean perch 3.8
Channel catfish	320	- -
Fathead minnow	224	1.7
Fathead minnow	2081	3.4
Fathead minnow	1189	5.4
geomean fathead minnow	821	fathead mean 3.5
Atlantic silverside	31	2.0

b. Aquatic Invertebrates

Acceptable data on aquatic invertebrates were very limited for ChemX. One acute study with the water flea, *Daphnia magna*, was available for freshwater arthropods (Mayer and Ellersieck 1985). Similarly, only one study was available with the estuarine pink shrimp, *Penaeus duorarum*, with sufficient data to calculate a dose-response slope, was available to represent saltwater crustaceans. To establish a toxicity distribution profile to estimate 5th percentile, 50th percentile, and 95th percentile sensitive invertebrates, a profile of pesticides in the same chemical class was used to determine where *Daphnia magna* typically falls in sensitivity. Four pesticides in the same chemical class as ChemX with a minimum of 5 species tested, including *Daphnia magna*, were used in the analysis. For these 4 chemicals, *D. magna* averaged the 25th percentile sensitive species with a range of from 5th to 50th percentile sensitive species, based on LC50s. Commercial Monte Carlo software (Crystal Ball Pro 4.0, Decisioneering Inc.) was used to estimate the 5th , 50th and 95th percentile invertebrate LC50s for ChemX, assuming a log normal distribution with the LC50 of *D. magna* at 25th percentile. The coefficient of variation was observed to be approximately constant at a value of 2, when examining the species sensitivities data for other pesticides in the same chemical class. Therefore, this same coefficient of variation was applied to the data when modeling the ChemX species sensitivity distribution. The mean and standard deviation for the Monte Carlo model were approximated by an iterative interpolation process in order to yield a 25th percentile estimate of LC50 at 29 ppb (measured LC50 for *D. magna*). The following table provides a summary of the commercial Monte Carlo software input parameters and subsequent output. Similar results could be obtained through direct calculation. It should be noted that toxicity data were available only for crustaceans and insects, and thus the species sensitivity curve for invertebrates does not include other invertebrate groups (e.g. molluscs, annelids). Lethality data on these other groups are generally not included in a pesticide risk assessment data package.

Table 7. Input Assumptions for Aquatic Invertebrate Species Sensitivity Distribution

Input Assumption: Lognormal distribution of LC50s, Daphnia 25th%ile species in sensitivity		
Daphnia	EC50 (ug/L)	29
	Mean	150
	Standard Deviation	300

Table 8. Output for ChemX Invertebrate Species Sensitivity Distribution

Percentile	EC50 (ug/L)
5%	8.83
25%	28.82
50%	68.91
75%	164.61
95%	563.13

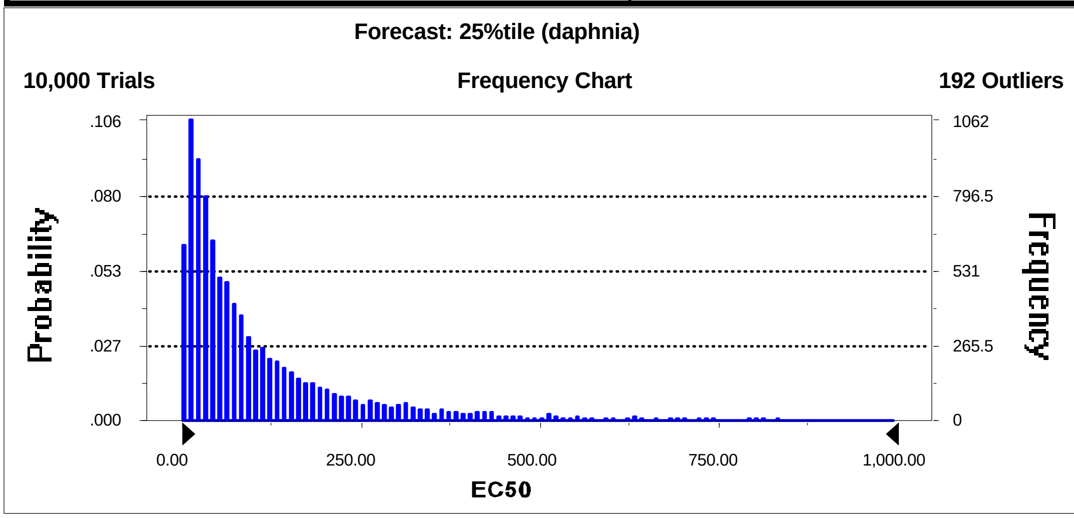


Figure 1. Distribution of Freshwater Invertebrate Sensitivities (EC50s) to Chem X Estimated through Monte Carlo Simulation

F. Routes of Exposure Considered in the Assessment

Due to the high solubility, low K_{ow}, and low Bioconcentration Factor, uptake from the water column was considered the only route of exposure for aquatic organisms in this assessment.

III. The Probabilistic Risk Assessment Model

A. General Model Overview

In refining the quotient-based risk assessment of the ChemX, the initial assessment was to screen the various label uses for risk and select specific ones for further analysis (refer to Section II. C). A key element in this analysis was estimating a 5^{th} percentile sensitive species of fish and aquatic invertebrates.

The next refinement was to determine a joint probability function from combining an exposure distribution derived from a PRZM-EXAMS model run using fixed, 36 year meteorological data and an acute toxicity dose response distribution derived from focal species analysis (refer to Section II. E. 1.) were combined and subjected to Monte Carlo analysis to derive a complementary cumulative distribution function.

The current PRZM-EXAMS model predicts the EEC's at ostensibly a 1-in-10 year probability, based on the temporal consideration of 36 continuous years of simulation from 1948 to 1983, using meteorological data. The full dose-response curve for each species or represented group/taxa indicated was employed in deriving the joint probability function. The dose-response curves were extrapolated based on the actual data for the species or created by Monte Carlo simulation of available data for the generic representatives (e.g., 5th percentile sensitive species).

This approach combines the exposure estimates with the estimates of biological effects expected at various concentrations. Therefore, the joint probability curves produced from these estimates describe the probability of an environmental concentration exceeding a concentration which would result in a quantitative estimate of the magnitude of a given detrimental biological effect such as mortality or reduced growth. The dose-response curve for an individual species can be considered to represent the percent probability of an individual being affected or the percent of the population that will be affected.

B. Exposure Modeling

The exposure assessment at Level 2 is intended to provide initial probabilistic estimates of exposure for vulnerable headwater environments across a wide range of geographical conditions as appropriate for product use. Currently, Tier 2 EEC assessments use a single site which represents a high-end exposure scenario from pesticide use on a particular crop or non-crop use site for multiple years (typically 36 years). In some cases, multiple exposure model runs are conducted to address different scenarios. The scenario or scenarios chosen are best professional judgement sites expected to produce runoff greater than would be expected at 90% of the sites for a given crop/use.

1. Exposure Model Overview

The Pesticide Root Zone Model (PRZM) simulates the movement of pesticides in the unsaturated soil, within and below the plant root zone, and extending to the water table using generally available input data that are reasonable in spatial and temporal requirements. EFED primarily uses PRZM as a runoff model. The model consists of hydrology and chemical transport components that simulate runoff, erosion, plant uptake, leaching, decay, foliar washoff and volatilization of a pesticide. In order to run PRZM, four types of input data are needed: meteorology, soil, hydrology and pesticide chemistry. Except for the pesticide chemistry, the input data were provided from the PIRANHA (Pesticide and Industrial Chemical Risk Analysis and Hazard Assessment, developed by Burns, et al., 1992) software package.

The Exposure Analysis Modeling System (EXAMS) was designed for rapid evaluation of the behavior of synthetic organic chemicals in aquatic ecosystems. From the chemistry of a compound, and the relevant transport and physical/chemical characteristics of the ecosystem, EXAMS computes (1) Exposure: the ultimate (steady-state) expected environmental concentrations (EECs) resulting from a specific pattern of (long term, time-invariant) chemical loadings, (2) Fate: the distribution of the chemical in the system and the fraction of the loadings consumed by each transport and transformation process, and (3) Persistence: the time required for effective purification of the system (via export/transformation processes) once the chemical loadings terminate. The model consists of transport and transformation processes. The transport process includes the results of advection and dispersion. The transformation process includes various chemical reactions, such as volatilization, hydrolysis, photochemical, redox, and microbial reactions and adsorption. In order to run EXAMS, three types of input data are needed: environment file, chemical file and loading file.

Currently, PRZM and EXAMS are linked for a refined estimation of pesticide concentration in surface water environment. PRZM 3.12 simulates the runoff and erosion from an agricultural field and EXAMS 2.97.5 simulates the fate in a receiving water body. The water body simulated is a static pond, adjacent to the crop of interest. The model yields an output of annual maxima distributions of instantaneous -peak, 96 hour, 21 day, 60 day, 90 day and yearly intervals.

2. Refinements of Level 2 Exposure Modeling

An approach to refining Level 2 exposure assessments used for the ChemX refined risk assessment was taken to attempt to address the uncertainties associated with model input parameters by various simulations with PRZM/EXAMS for a single scenario, as outlined in the model scenario matrix section below.

Additionally regional variations in expected outcomes were addressed for the usage of ChemX on potatoes, by modeling estimated concentrations for different areas of the country assessed to have high usage on potatoes based on BEAD analyses.

C. Effects Assessment

Acute toxicity values used in this assessment were drawn from the recalculated values (see section II.E.). Freshwater fish and estuarine/marine fish were considered separately. A normal distribution of log LC50s and log standard deviations was assumed in extrapolating 5th percentile and 50th percentile toxicity values for freshwater fish. Data for estuarine/marine fishes was limited to the Atlantic silverside and these data were used without further extrapolation. In addition to the percentile extrapolations as noted, bluegill sunfish and rainbow trout were also included. These two species are the most commonly tested species to support pesticide registrations and, therefore, considered important to include in the assessment to aid in interpretation.

Acute toxicity data were very limited for invertebrates and the data available for *Daphnia magna* were not sufficient to estimate a slope for the dose-response curve. The data with the pink shrimp for ChemX were used to estimate a slope, and due to the absence of other data this value was used for freshwater invertebrates. The 5th and 50th percentile species in invertebrate sensitivity were extrapolated based on the sensitivity of *D. magna* to pesticides in the same class as ChemX (see section II.E. 1.b.). The mortality of the 5th and 50th percentile freshwater invertebrates was estimated. The mortality in the 95th percentile species in sensitivity (less sensitive) was not estimated as it was expected to have a toxicity outside the range of appreciable risk.

Table 9. Aquatic Species Toxicity Data

Species	LC50 (EC50)	Slope
Freshwater Fish		
5th percentile species	81 [2]	5.5 [2]
Bluegill sunfish	104 [1]	6.8 [1]
Rainbow trout	306 [1]	3.2 [1]
50th percentile species	295 [2]	5.5 [2]
Estuarine fish		
Atlantic silverside	31 [1]	2.1 [1]
Freshwater invertebrate		
Daphnia magna	33 [1]	5.8 [3]
5th percentile species with Daphnia 25th percentile species	9	5.8 [3]
50th percentile species with Daphnia 25th percentile species	69	5.8 [3]
Estuarine invertebrate		
Pink shrimp	7 [1]	5.8 [1]

[1]From actual data
[2]From distribution of freshwater fish data
[3]From the pink shrimp dose-response data
[4]From the distribution of invertebrate data for pesticides in the same chemical class

For evaluation of chronic effects, the actual data (NOEC and LOEC) were used for *D. magna* as a representative aquatic invertebrate and rainbow trout as a typical fish. However, an extrapolated value (ENEC) was used for the bluegill sunfish. The bluegill sunfish was the most sensitive tested fish for acute exposures but it was not tested in a longer term study. An Estimated No Effect Concentration (ENEC) was determined for the bluegill sunfish using the acute to chronic ratio calculated for rainbow trout.

D. Risk Assessment Model

1. Acute Risk Prediction Approach

Two-dimensional Monte Carlo analysis was used to estimate mortality in fish and invertebrates following peak instantaneous exposure to ChemX applied at the maximum application rates for the crops noted above. Peak exposures are considered appropriate because they represent worst case and information on “time to event” are generally lacking. In the case of ChemX, the 24-hour LC50 for fish were identical to the corresponding 96-hour LC50 for 2 of the species tested (coho salmon and lake trout) and within the 95% confidence limits of the 96-hour LC50 in 10 of the 14 tests and all but one of the 10 species tested (rainbow trout). This indicates that all or most of the mortality occurs in the first 24 hours after exposure. Therefore, the available evidence supports the concept that the lethal effects of ChemX to aquatic organisms occur very rapidly.

Some definitions useful for the interpretation of the results of a probabilistic analysis include that of variability and uncertainty. The following explanations were taken from the US EPA document entitled Guiding Principles for Monte Carlo Analysis (1997). “Variability refers to observed differences attributable to *true heterogeneity* or diversity in a population or exposure parameter. Sources of variability are the result of natural random processes and stem from environmental, lifestyle, and genetic differences among humans. Examples include human physiological variation (e.g., natural variation in bodyweight, height, breathing rates, drinking water intake rates), weather variability, variation in soil types and differences in contaminant concentrations in the environment. Variability is usually not reducible by further measurement or study (but can be better characterized).” ...“Uncertainty refers to *lack of knowledge* about specific factors, parameters, or models. For example, we may be uncertain about the mean concentration of a specific pollutant at a contaminated site or we may be uncertain about a specific measure of uptake (e.g., 95th percentile fish consumption rate among all adult males in the United States). Uncertainty includes *parameter uncertainty* (measurement errors, sampling errors, systematic errors), *model uncertainty* (uncertainty due to necessary simplification of real-world processes, mis-specification of the model structure, model misuse, use of inappropriate surrogate variables), and *scenario uncertainty* (descriptive errors, aggregation errors, errors in professional judgment, incomplete analysis).”

An example of variability pertaining to this risk assessment is the natural variability in different species’ sensitivities to ChemX. There may also be uncertainty about the true LC_{50} for a given species at a given age, within a laboratory, if the toxicity test has been insufficiently replicated. There are also uncertainties regarding sensitivities of various species at different ages, nutritional, and disease states, as well as uncertainty regarding the accuracy of laboratory toxicity estimates to applied to field populations. These uncertainties may be reduced through further laboratory and field testing, variability will not be. There are a number of other sources of variability and uncertainty in this risk assessment, particularly regarding exposure estimates.

In a conventional Monte Carlo analysis, the risk assessor uses computer simulation to estimate how natural variation in the inputs to a exposure/risk model affect the model's output. The computer is used to estimate, through simulation, what could not be calculated easily or routinely in any other straight-forward manner. In a conventional Monte Carlo analysis, the assessor acts as if the variability in each of the model's inputs are known absolutely with no uncertainty. This is never the case, especially for environmental assessments where data are often scarce and often of less than ideal quality. A conventional Monte Carlo analysis cannot account for the uneven quality of the data inputs.

A 2-dimensional (2-D) Monte Carlo analysis is an attempt to quantitatively recognize that the inputs to an exposure/risk model have varying degrees of uncertainty associated with them and that the model's output should reflect or capture this uncertainty. A 2-D assessment may be best thought of as repeated Monte Carlo analyses in which the difference between successive Monte Carlo runs reflects uncertainty in the input distributions.

In a 1-D analysis, the effect of variation in the inputs to the model on predicted exposures or risks is examined. For a 1-D analysis, the statistical distribution characterizing each input is usually based on best estimates or expert judgment. In a 2-D analysis, the effect of both variation and uncertainty on predicted exposures or risks is evaluated. For a 2-D analysis, each input is characterized by a statistical distribution and confidence about its parameters.

The results of a 2-D analysis can be significantly more informative. A 1-D analysis yields estimates of key statistics of the model's output. For example, a 1-D analysis would provide estimates of the mean, 95th and 99th percentile exposures, without any sense of how robust those estimates might be. In contrast, in a 2-D analysis, quantitative confidence bounds (generally termed credible bounds in a 2-D analysis) to those key statistics are produced, as well as a quantitative characterization the robustness of the statistics .

A 2-D analysis can sometimes be more difficult than a conventional (or 1-D) analysis, both in terms of effort, software and computational time. There can also be challenges in presenting the technique and findings to groups with limited technical backgrounds. Technical details about the Monte Carlo analyses are presented in the appendix.

a. Acute Risk Estimates

Acute effects data were fitted to a dose-response curve, based on standard EPA usage of log-Probit fits to 96 hour acute toxicity data. SAS software (version 6.12) was used to fit the effects data.

Exposure data were generated through the use of PRZM 3.12/EXAMS 2.97.5, as described above in sections IIIA and B. The peak concentration (annual maxima) estimates for each year modeled were used in the acute risk simulations. Typically, 36 years of model data are used. Peak concentrations were used in 2 manners: (1) The peak exposure model-generated data was fit to a theoretical distribution using *ExpertFit*™ Software *(*version 1.37, Averill M. Law & Associates). The distribution that best fit the data was selected within *ExpertFit*™, based on a heuristic procedure used to rank fits. The theoretical distribution with the best fit was then used, along with the effects data, in a commercial software-based (Crystal Ball) Monte Carlo simulation, to estimate risk of mortality; (2) The peak exposure model-generated data was employed in an empirical method, via bootstrapping. The empirical distribution was used along with the effects data in a C-program written by an EPA analyst to estimate risk of mortality.

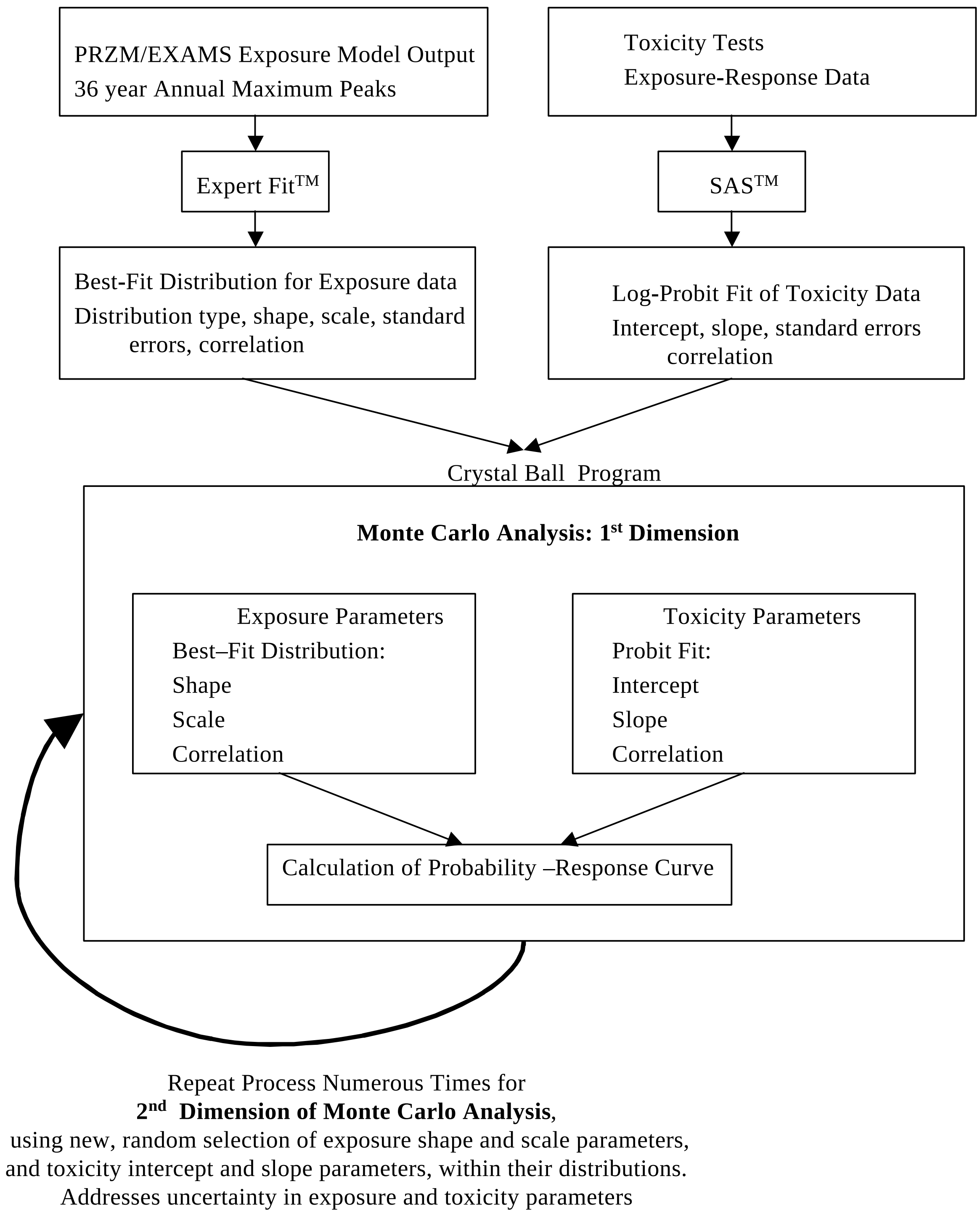
Both the commercial program usage and the EPA C-program usage are discussed in detail below. The two sets of analyses, theoretical and empirical, were performed for several scenarios in order to evaluate the impact of fitting the exposure model output to a standard distribution versus using the exposure model output more directly, in an empirical fitting method. The two methods of analysis were also evaluated for their efficiency and ease of use for future probabilistic risk assessments. The overall analysis provides an estimates of percent mortality in a population. The risk estimates are based on acute effects in the laboratory and estimated exposure concentrations based on exposure simulation modeling of a number of usage scenarios via PRZM/EXAMS. Therefore, these risk estimates do not directly take into account uncertainties such as laboratory-to-field sensitivity differences and uncertainties regarding the difference between model-estimated concentrations and actual environmental concentrations.

i. Simulations Using a Theoretical Distribution: Acute Risk

Estimates of acute risk to fish and invertebrates were based on the use of a commercial Monte Carlo software package. A flowchart of the process for completing this analysis is shown in figure 2. The commercial Monte Carlo software worksheet was programmed to produce 2-dimensional Monte Carlo analyses, based on the input of toxicity and environmental exposure data. A software worksheet example is given in the appendix. Model input parameters, including best-fit distributions with associated parameter estimates for the exposure modeling output, as well as toxicity input parameters are also given in the appendix.

The first dimension of the Monte Carlo analysis involved conducting a series of calculations of the exposure and effects data to estimate percent mortality for the species modeled. At the initiation of each first dimension, or inner loop, of the Monte Carlo analysis, a unique set of values for the slope and intercept of the effects dose-response curve, as well as a unique set of values for the exposure best-fit shape and scale parameters was selected randomly by the Commercial Monte Carlo program. The intercept, slope, shape and scale parameters themselves were assumed to be normally distributed, with best estimates and standard deviations determined by the external *ExpertFit*™ and SAS programs. The exposure concentration selected was then entered into the equation for the dose-response line, and an estimated individual risk was produced. The random selection of exposure probability and associated risk estimate was conducted 5000 times for each unique set of input parameters. The second dimension, or outer loop of the Monte Carlo simulation was then completed by repeating the process 250 times for 250 unique sets of the four model parameters described above. (250 is the maximum number of outer loops that can be performed using commercial Monte Carlo program software.) The outer loop of the Monte Carlo analysis permitted an evaluation of the uncertainty in the mortality predictions based on uncertainty regarding the exact values for each of the parameters in the model, based on the model fits to the data. Individual calculated risks were multiplied by one hundred to estimate the percent mortality in a large fish population.

Figure 2. Two-Dimensional Monte Carlo Approach Using a Theoretical Distribution



ii. Simulation Using an Empirical Distribution: Acute Risk

A program was written in C by an EPA analyst to perform an identical procedure as the commercial Monte Carlo program analyses as described above, but with the use of empirical data for exposure peaks, in lieu of best-fit exposure data. In this program, minimum and maximum exposure concentrations beyond the range of exposure peaks produced through PRZM/EXAMS modeling were entered. The minimum possible exposure peak was set to zero, based on a best professional judgement that in some years there may be no exposure to the pond from drift, due to the wind blowing in a direction away from the pond modeled, coupled with a lack of runoff. A linear extrapolation of the data from the lowest peak to zero was made, to estimate concentrations below the lowest observed peak. An exponential tail for the high end of the exposure distribution, based on the three highest modeled peaks, was included in the program. A maximum for the exponential tail was set. A general recommended approach for selecting the maximum was derived for the current, as well as future, risk assessments. The maximum selected is recommended to be the lower of ten times the maximum peak estimated, or the solubility limit. The solubility of ChemX in water is 700 ppm, greatly exceeding any maximum estimated peak for any crop. Therefore, an estimated maximum peak of 10 times the modeled peak was selected as a more likely potential maximum for this risk assessment. The inner loop of the Monte Carlo analyses was performed 2500 times and the outer loop 2500 times for the Ohio Corn scenario. For all other scenarios analyzed using this program, 2500 inner loops were performed and 5000 outer loop simulations. In the outer loop, the exposure data was resampled with replacement (bootstrapping) to simulate uncertainty in the exposure data. The effects data were also randomly sampled within their fitted Probit distributions in the outer loop, to simulate uncertainty regarding the slope and intercept of the dose-response curve parameters. Individual calculated risks were multiplied by one hundred to estimate the percent mortality in a large fish population.

2. Chronic Risk Prediction Approach

Estimates of chronic risk were based on a Level of Concern exceedence approach. Currently, current chronic tests are evaluated using a hypothesis testing approach, yielding estimates of No-Observed-Effect-Concentrations (NOECs) and Lowest-Observed-Effect-Concentrations (LOECs), which were used in this refined assessment. The frequency of exposure model predictions exceeding a NOEC and LOEC was calculated for a number of time intervals and usage scenarios, for freshwater species for which the data were available. Species examined were rainbow trout, and the invertebrate *Daphnia magna*. There were no chronic core studies completed on the most sensitive species, bluegill, so a chronic NOEC was estimated for bluegill based on an acute-to-chronic ratio approach, and a Estimated No-Effect Concentration (ENEC) was used in the chronic exceedence frequency analysis for this species. The lack of a robust dose-response experimental design and associated analysis in current chronic toxicity tests, in combination with resource constraints, precluded a probabilistic dose-response approach for chronic effects.

a. Chronic Risk Estimates

Commercial Monte Carlo software was used to assess potential chronic effects in an exceedence frequency, wherein the distribution of potential exposures was compared to a point estimate of toxicity. The frequency of exposures exceeding chronic NOECs and LOECs (ENEC for bluegill) was analyzed for several time intervals, in an Level of Concern exceedence probability approach. Currently there is an inability to detect the potential latent effects of brief exposures, given the current chronic toxicity test paradigm. Therefore, NOECs and LOECs were compared to a sequence of time intervals: peak yearly estimated concentrations, and 96 hour, 21 day and 60 day yearly running average maxima. These analyses were performed for corn, cotton, potatoes, and grapes, using the standard scenarios at maximum and typical application rates. Two sets of chronic analyses were performed for comparison. One set of analyses was based on a fitted peak exposure distributions via *Expert Fit*™ software. The second set was based on exposure distribution fits selected through the commercial Monte Carlo software facility for distribution fitting, which was done for the series of time intervals noted above (peak, 96 hour, 21 day, 60 day).

i. *Expert Fit*™ Exposure Distribution Selection: Chronic Risk Following Peak Exposure
The distributions used for calculating chronic Level of Concern exceedence frequency were the same as that used for the commercial Monte Carlo software simulations for acute mortality for each scenario, based on peak exposure. In the chronic effects evaluation, a probability was randomly selected and an exposure concentration was calculated through inversion of the best fit distribution, based on 10,000 iterations. The frequency of exceeding the NOECs/LOECS/ENEC for fish and invertebrates was then directly read from the commercial Monte Carlo software chart for the simulated peak exposure distribution.

ii. Theoretical Exposure Distribution Selection: Chronic Risk at Several Time Intervals
The second set of chronic risk evaluations were completed based on the comercial Monte Carlo program's internal distribution fitting capability. The yearly maxima for peak, and 96 hour, 21 day and 60 day running averages were fit, and an exposure simulation of 10,000 iterations was completed. The frequency of exceeding the NOECs/LOECs/ENEC for fish and invertebrates was then directly read from the commercial Monte Carlo software chart for the various time intervals. The values based on the theoretical distributions are those reported in the results, because the results based on distributions derived via the *Expert Fit*™ software were not significantly different, and were limited to peak exposures for this analysis.

IV. Model Scenario Matrix

A. Exposure Scenario Selection

The rationale for exposure scenarios selected for probabilistic analysis were based on two concepts: (1) As a refined risk assessment it would be most useful to assess the same exposure scenarios modeled in the deterministic assessment, in order to clearly identify the differences in expected outcomes when moving from deterministic to probabilistic methods, and (2) examination of additional scenarios would provide a more comprehensive understanding of the potential ecological risks. Thus, as an initial step, corn, cotton, potatoes and grapes, based on standard EFED scenarios, were selected for probabilistic analyses. Maximum use rates were selected to be modeled first. Due to the calculated low probability of acute effects on fish at the maximum ChemX use rates, lower use rates were not modeled for acute effects. Corn and cotton were selected because of the high usages of ChemX in terms of acres of crop treated. Potatoes were selected to represent a less prevalent usage, but higher peak risk than corn or cotton, as determined in the deterministic risk assessment (see table in section II.C.). Usage of ChemX on grapes is lower than the above crops, in terms of total acres treated, but the risk to aquatic species was determined to be higher, and so grapes were also selected as a model scenario.

B. Exposure Model Matrix

Iowa was selected for use as a test case for examining model sensitivity to variation in selected model input parameters due to the high usage of ChemX on corn in Iowa, based on BEAD data, and its availability as a standard corn scenario. The scenario chosen was a corn field in Pottawottamie County, Iowa, within the Major Land Resource Area (MLRA) 107 for Iowa and Missouri Deep Loess Hills. The standard modeling setting assumes a 10-hectare corn field draining into a 1-hectare static pond, 2-meter deep with no outlet. The soil selected is Marshall silty clay loam soil, which belongs to “B” hydrologic group soil and is expected to produce moderate runoff and erosion. Data for the Marshall silty clay loam was taken from the PIC (PRZM Input Collator) database in PIRANHA and the 1987 National Resources Inventory. USLE soil loss ratios are based on plant cover and USDA Paper 537 (United States Soil Conservation Service, 1972). Weather data was taken from weather station W14943 in Sioux City, Iowa. The ChemX was applied twice at a rate of 1.0 lb a.i./ac May 5 and May 20 of each year during the simulation period of 1948 to 1983.

To estimate the sensitivity of the predicted outcomes regarding mortality following acute exposures, specific exposure modeling parameters that were expected to have a substantial effect on exposures estimates, based on best professional judgement, were varied within individual PRZM/EXAMS simulations for Iowa corn. These parameters included pH of the receiving water body, soil aerobic metabolism rates, and the size of the treated field relative to the size of the water body receiving runoff from the field. The selection of pH as a potentially sensitive parameter was based on the sensitivity of ChemX hydrolysis rates to pH. ChemX hydrolysis half-lives vary from nearly a year at pH 6.2, to approximately one month at pH 7, to less than one day at pH 9. (All rates were for 25-28^{O}C). Therefore, pH was expected to have a substantial impact on estimated environmental concentrations The selection of soil aerobic metabolism was based on PRZM/EXAMS model sensitivity to soil aerobic metabolism rate, and was used to examine the differences in output when inputting the mean soil aerobic metabolism half-life and the 90th percentile value.

The field to pond size ratio was selected for inclusion in sensitivity analyses because of the wide differential between the field to pond size ratio typically used in all EFED PRZM/EXAMS modeling, 10:1, and that suggested for other areas of the country, such as Iowa, where the ratio may be as high as 120:1. The range of field to pond sizes used for modeling ChemX usage in Iowa was based on a USDA Soil Conservation Service Publication outlining recommendations for farm pond construction (USDA, 1982). This publication outlines approximate optimal sizes of drainage area (in acres) required for each acre-foot of storage in an excavated pond for different areas of the country. The recommended dimensions given in the USDA publication were designed to yield a pond sufficiently large to permit maintenance of water in the pond during droughts, yet small enough not to require overflow structures to bypass excess runoff during storms. The field to pond size ratio typically used in EFED PRZM EXAMS modeling is based on a Mississippi drainage area factor of 2 acres for a recommended acre-foot minimum depth of 6 feet for a 1 acre pond, yielding a drainage area or field size of 12 acres for a one acre pond. That number has been rounded to 10:1 for EFED standard modeling purposes. In assessing the Iowa scenario, the recommended drainage area factors for Iowa vary from 8 to 20. An overlay of the USDA Soil Conservation publication figure on the BEAD ChemX usage data, was used in the field to pond size ratio selections. In order to simplify the exercise, we maintained the modeled pond depth at 6 feet (USDA actual recommended value of 7-8 feet), and varied the field size from a low of 8 acres per acre foot, yielding a field to pond size ratio of 48:1 (8 field acres per 1 acre, 6 foot deep pond, giving 48:1), though an estimated average recommended field to pond size ratio of 60:1 (10 field acres per pond acre foot), to a maximum of 120:1. The matrix of exposure variables used to examine model sensitivity to these parameters is given below in table 10.

To adjust the field-to-pond (FTP) ratio, as indicated in the Matrix of Exposure Variables for PRZM/EXAMS Model sensitivity Analysis, the values of 48, 60 and 120 were used to describe the small, medium and large FTP scenarios. The input parameter, AFIELD, defines the area of field or plot in hectares. The different FTP value for AFIELD were entered, and PRZM wrote the FTP value to the annual output files. When EXAMS read the loading information from the PRZM annual output file, the FTP information was transferred and used in EXAMS computation to reflect the desired FTP.

To simulate the different pond pH scenarios, the pH and pOH values in the EXAMS pond file were changed from the standard pH 7 scenario. The hydrolysis reaction simulated in EXAMS is a combination of acidic, neutral and basic catalytic reactions. As the following equation shows, the overall hydrolysis rate constant (K_{H2O}) is the results of three individual catalytic reactions.

$$K_{H2O} = Kah\,[H^+] + Knh + Kbh\,[OH^-]$$

Based on the results of the laboratory hydrolysis study, there were three tests done at different pH values (6.2, 7.0, and 9.0). The tests report the half-life value. The hydrolysis reaction rate constant was calculated by converting the half-life value with the following equation.

$$K_{H2O} = \ln(2) \div T½$$

By combining the three hydrolysis rate constants equations, a linear matrix was used as shown below. With a readily available matrix conversion program, the value of Kah, Knh, and Kbh was estimated.

$$K_{H2O}\,@6.2 = Kah\,[H^+]@6.2 + Knh + Kbh\,[OH^-]@6.2$$

$$K_{H2O}\ @7.0 = \quad Kah\ [H^{+}]@7.0 \quad + \quad Knh \quad + \quad Kbh\ [OH^{-}]@7.0$$

$$K_{H2O}\ @9.0 = \quad Kah\ [H^{+}]@9.0 \quad + \quad Knh \quad + \quad Kbh\ [OH^{-}]@9.0$$

The values of Kah, Knh, and Kbh were then input into the EXAMS chemical file. During the EXAMS simulations, the program read the pond pH and pOH and then computed the overall hydrolysis rate constant based on the rate constants stored in the chemical file.

Table 10. Matrix of Exposure Variables PRZM/EXAMS Model Sensitivity Analysis. Used for largest use crop (Corn) in Iowa.

Scenario	pH	Soil Aerobic metabolism rate	Field:Pond Size Ratio
1	pH 6.2	90% value	Low= 48 A/A
2	pH 6.2	90% value	Ave= 60 A/A
3	pH 6.2	90% value	High= 120 A/A
4	pH 6.2	Mean value	Low = 48 A/A
5	pH 6.2	Mean value	Median= 60 A/A
6	pH 6.2	Mean value	High=120 A/A
7	pH 7	90% value	Low= 48
8	pH 7	90% value	Median = 60
9	pH 7	90% value	High = 120
10	pH 7	90 % value	Standard scenario = 10 A/A
11	pH 7	Mean value	Low= 48
12	pH 7	Mean value	Median = 60
13	pH 7	Mean value	High = 120
14	pH 7	Mean value	Standard Scenario = 10 A/A
15	pH 9	90% value	Low = 48
16	pH 9	90% value	Median= 60
17	pH 9	90% value	High = 120
18	pH 9	Mean value	Low = 48
19	pH 9	Mean value	Median = 60
20	pH 9	Mean value	High = 120

V. Results

A. Acute effects

The analysis included simulations performed with a commercial Monte Carlo software using a "best fit" theoretical distribution selection via *Expert Fit*™ Software for the exposure profile generated by PRZM/EXAMS runs for the scenario selected. The analysis also included, in some cases, parallel empirically derived bootstrap simulations from the same exposure model runs. For fish, the estuarine Atlantic silverside, a generic 5th percentile freshwater sensitive species, the bluegill sunfish, the rainbow trout, and a generic 50th percentile freshwater sensitive species were assessed in a joint probability function with exposure. For invertebrates, the toxicity data of *Daphnia magna*, the estimated toxicity data of a generic 5th percentile sensitive freshwater invertebrate with *D. magna* as a 25th percentile sensitive freshwater invertebrate, the estimated toxicity data of a generic 50th percentile freshwater invertebrate with *D. magna* as a 25th percentile sensitive freshwater invertebrate, and the toxicity data of the estuarine pink shrimp were combined in a joint probability function with the estimated exposure. The estimated toxicity of a 5th percentile sensitive freshwater invertebrate with *D. magna* as a 50th percentile sensitive freshwater invertebrate was included for the Ohio corn analysis. The following tables provide the percent mortality expected to these selected representative species for a 5th percentile, median, mean, and 95th percentile risk outcomes. Additionally, in the case of Iowa corn, the effects of pH, aerobic metabolism rate, and the field size to pond area ratio on the exposure output and estimated acute risk outcomes were evaluated (see section 2). In this case, only rainbow trout and *D. magna* were used for the effects component in the joint probability function analysis. The tables are organized in the following order for each crop: acute risk to fish (theoretical model), acute risk to fish (empirical model), acute risk to invertebrates (theoretical model), and acute risk to invertebrates (empirical model). Mean estimates are provided for various ranges, with 5th and 95th% confidence bounds given in parentheses. The results described in the text are those generated by the empirical model (EPA program), the second table in each set, when that information was available. When only the theoretical model (commercial Monte Carlo software-based) results were available, those are the data listed in the descriptive text.

1. Standard Scenarios Modeled in the Deterministic Risk Assessment

a. Ohio Corn

Table 11. Ohio Corn: Estimated Percent Mortality in Fish Following Acute Exposure to ChemX. Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Atlantic silverside	5^{th} percentile species	Bluegill sunfish	Rainbow trout	50^{th} percentile species
5^{th} percentile	24 (15-33)	<1 (0-1)	<1 (0- <1)	<1 (0- <1)	0 (0-0)
median	31 (22-40)	1 (<1-4)	<1 (0- <1)	<1 (0-1)	<1 (0-<1)
mean	32 (23-41)	2 (<1-8)	<1 (<1- <1)	<1 (<1-1)	<1 (0-<1)
95^{th} percentile	44 (35-55)	6 (<1-32)	<1 (0- 1)	1 (<1-2)	<1 (0-<1)

Table 12. Ohio Corn: Estimated Percent Mortality in Fish Following Acute Exposure to ChemX. Empirical Model Simulations: Empirical Distribution for Exposure. 6.25 Million Simulations

	Atlantic silverside	5^{th} percentile species	Bluegill sunfish	Rainbow trout	50^{th} percentile species
5^{th} percentile	25 (17-33)	<1 (0-1)	<1 (0- <1)	<1 (0- <1)	0 (0- <1)
median	31 (22-40)	1 (<1-3)	<1 (0- <1)	<1 (0- 1)	<1 (0- <1)
mean	32 (24-40)	2 (<1-8)	<1 (<1- 1)	<1 (0- 1)	<1 (0- <1)
95^{th} percentile	49 (36-63)	8 (<1-40)	<1 (0- 1)	<1 (<1- 2)	<1 (0- <1)

In the Ohio corn scenario, the analysis based on the theoretical model and the empirical model distributions were closely matched. Estuarine Atlantic silverside exposed to ChemX, at concentrations equivalent to those estimated for farm ponds, would be expected to experience significant mortalities. The best estimate of expected mortality would be 32% (95 % confidence bounds of 24-40%), across the range of exposure concentrations and silversides sensitivities. 95% of the time, mortality would be expected to exceed 25% (17-33%). 5% of the time, mortality would be expected to exceed 49% (39-63%). The estuarine fish was included in the Ohio corn analysis for several reasons: for comparison to the RQ-based deterministic estimates of risk given in the deterministic assessment, to represent more sensitive fish potentially present in the corn scenario, and also to represent potential sensitivities in estuarine fish (relative to freshwater fish) present in other corn-growing regions. Freshwater fish would generally not be expected to show any significant mortality. Fish of high sensitivity (5^{th} percentile), would only be expected to experience 2% mortality (<1-8 %), but 5% of the time would incur somewhat higher mortality, typically exceeding 8% (<1-40%).

Table 13. Ohio Corn: Estimated Percent Mortality in Invertebrates Following Acute Exposure to ChemX.
Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Daphnia	5th percentile species w/Daphnia 25th%tile	50th percentile species w/Daphnia 25th %tile	5th percentile species w/Daphnia 50th %tile	Shrimp
5th percentile	2 (<1--6)	71 (11-100)	2 (0-9)	100 (100-100)	94 (86-99)
median	7 (1-26)	82 (30-100)	3 (0-15)	100 (100-100)	98 (94-100)
mean	11 (1-33)	82 (34-100)	4 (<1-20)	100 (100-100)	97 (93-100)
95th percentile	31 (4-78)	95 (77-100)	8 (<1-52)	100 (100-100)	100 (99-100)

Table 14. Ohio Corn: Estimated Percent Mortality in Invertebrates Following Acute Exposure to ChemX.
Empirical Model Simulations: Empirical Distribution for Exposure. 6.25 Million Simulations

	Daphnia	5th percentile species w/Daphnia 25th%tile	50th percentile species w/Daphnia 25th %tile	5th percentile species w/Daphnia 50th %tile	Shrimp
5th percentile	2 (<1-7)	75 (8-100)	2 (0-8)	100 (100-100)	94 (86-99)
median	7 (1-22)	84 (23-100)	2 (0-15)	100 (100-100)	98 (92-100)
mean	11 (2-27)	83 (28-100)	4 (<1-18)	99 (99-100)	96 (91-98)
95th percentile	41 (5-89)	97 (81-100)	10 (<1-49)	100 (100-100)	100 (99-100)

As seen with the fish, the analyses based on the theoretical model and the empirical model distributions were closely matched for invertebrates. Invertebrate mortality, though, can be expected to be relatively substantial for species with sensitivities close to that of *D. magna*. For *D. magna* with a best estimate of 11% mortality (2-27%) was estimated. Five percent of the time, 41% mortality (5-89%) would be expected. Very sensitive freshwater invertebrates would be expected to have a mortality rate of 83% (28-100%). Estuarine invertebrates exposed to concentrations generally predicted for farm ponds in Ohio would be expected to suffer very high mortality, 96% (91-98%).

b. Mississippi Cotton

Table 15. Mississippi Cotton: Estimated Percent Mortality in Fish Following Acute Exposure to ChemX
Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Atlantic silverside	5th percentile species	Bluegill sunfish	Rainbow trout	50th percentile species
5th percentile	2 (<1-6)	0 (0-0)	0 (0-0)	<1 (0- <1)	0 (0-0)
median	8 (2-15)	<1(0- <1)	0 (0-0)	<1 (0- <1)	0 (0-0)
mean	16 (8-30)	4 (<1-17)	3 (<1-18)	2 (<1-9)	2 (<1-15)
95th percentile	56 (24-100)	26 (<1-100)	17 (0-100)	8 (0-84)	12 (0-100)

Table 16. Mississippi Cotton: Estimated Percent Mortality in Fish Following Acute Exposure to ChemX
Empirical Model Simulations: Empirical Distribution for Exposure. 12.5 Million Simulations

	Atlantic silverside	5th percentile species	Bluegill sunfish	Rainbow trout	50th percentile species
5th percentile	<1 (0- <1)	0 (0-0)	0 (0-0)	<1 (0-0)	0 (0-0)
median	6 (1-14)	0 (0-0)	0 (0-0)	<1 (0- <1)	0 (0-0)
mean	10 (6-16)	1 (<1-4)	<1 (0- 1)	<1 (<1- <1)	<1 (0- <1)
95th percentile	40 (20-65)	4 (<1-26)	<1 (0-1)	<1 (0-2)	<1 (0- <1)

Like the Ohio corn scenario, the analysis for Mississippi cotton based on the theoretical model and the empirical model distributions were generally similar in their mean estimates. However, there were differences in the tails of the distributions, particularly with the 95th percentile estimates (lower probability events). The difference in the tails of the distributions for the two models may have been due to the fact that the fitted exposure distribution used in the theoretical model had no upper bound, or to the goodness of fit in the tails of the selected theoretical distribution. Also, as seen in the Ohio situation, estuarine fish can be expected to suffer significant mortality where concentrations in their habitat resemble those modeled for ponds. Freshwater fish would generally not be expected to show significant mortality. Fish of high sensitivity (5th percentile), would only be expected to experience 1% mortality (<1-4%), but 5% of the time they would potentially incur higher mortality rates (4% , with confidence limits of <1-26%), based on the empirical model runs.

Table 17. Mississippi Cotton: Estimated Percent Mortality in Invertebrates Following Acute Exposure to ChemX
Theoretical Model Simulations. Fitted Distribution for Exposure. 1.25 Million Simulations

	Daphnia	5^{th} percentile species w/Daphnia 25^{th}%tile	50th percentile species w/Daphnia 25^{th} %tile	Shrimp
5^{th} percentile	0 (0- <1)	11 (0-77)	<1 (0- <1)	2 (0-10)
median	<1(0- <1)	34 (<1-99)	<1 (0- <1)	35 (9-65)
mean	8 (8-27)	43 (8-95)	4 (<1-18)	45 (32-60)
95^{th} percentile	52 (2-100)	95 (65-100)	25 (0-100)	99 (95-100)

Table 18. Mississippi Cotton: Estimated Percent Mortality in Invertebrates Following Acute Exposure to ChemX
Empirical Model Simulations: Empirical Distribution for Exposure. 12.5 Million Simulations

	Daphnia	5^{th} percentile species w/Daphnia 25^{th}%tile	50^{th} percentile species w/Daphnia 25^{th} %tile	Shrimp
5^{th} percentile	0 (0-0)	2 (0-5)	<1 (0-0)	<1 (0- <1)
median	<1 (0- <1)	28 (0-99)	<1 (0- <1)	21 (1-50)
mean	4(<1-9)	33 (4-83)	2 (<1-5)	35 (24-47)
95^{th} percentile	27 (<1-89)	89 (30-100)	7 (0-42)	98 (90-100)

As seen with Ohio corn, invertebrate mortality can be expected to occur for species with sensitivities close to that of *D. magna* under high exposure and sensitivity conditions. Very sensitive freshwater invertebrates could be expected to incur mortality of 33% (4-83%), with infrequent high morality events of 89% (30-100%) occurring 5% of the time, based on the empirical model analyses. Estuarine invertebrates exposed to concentrations generally predicted for farm ponds in Mississippi would be expected to suffer high mortality, 35% (24-47%). Mortality rates of up to 100% would be expected to occur approximately 5% of the time.

c. Maine Potatoes

Table 19. Maine Potatoes: Estimated Percent Mortality in Fish Following Acute Exposure to ChemX
Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Atlantic silverside	5th percentile species	Bluegill sunfish	Rainbow trout	50th percentile species
5th percentile	36 (26-45)	1 (<1-7)	<1 (0- <1)	<1 (0-1)	<1 (0-<1)
median	42 (32-52)	3 (<1-16)	<1 (0- <1)	<1 (<1-1)	<1 (0-<1)
mean	43 (33-53)	5 (<1-21)	<1 (<1-1)	<1 (<1-1)	<1 (0-<1)
95th percentile	56 (44-68)	12 (<1-51)	1 (<1-4)	1 (<1-4)	<1 (0- <1)

Table 20. Maine Potatoes: Estimated Percent Mortality in Invertebrates Following Acute Exposure to ChemX
Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Daphnia	5th percentile species w/Daphnia 25th%tile	50th percentile species w/Daphnia 25th %tile	Shrimp
5th percentile	15 (1-38)	90 (49-100)	4 (0-18)	99 (94-100)
median	28 (3-66)	95 (71-100)	6 (0-31)	99 (97-100)
mean	30 (4-66)	95 (72-100)	7 (<1-35)	99 (97-100)
95th percentile	55 (11-95)	99 (95-100)	15 (<1-60)	100 (100-100)

In the scenario for potatoes grown in Maine, freshwater fish can be expected to experience little mortality except for the most sensitive species in high exposure conditions. The mortality for the most sensitive fish species would be expected to be 5% (<1-21%), but could infrequently be as high as 12% (<1-51%). Invertebrates on the other hand can be expected to suffer significant mortalities. Species similar to *D. magna* in sensitivity to ChemX would be expected to experience 30% mortality (4-66%), with occasional levels attaining 55% (11-95%). Sensitive species would routinely experience very high levels of mortality(in the range of 100%).

d. California grapes

Table 21. Grapes: Estimated Percent Mortality in Fish Following Acute Exposure to ChemX
Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Atlantic silverside	5th percentile species	Bluegill sunfish	Rainbow trout	50th percentile species
5th percentile	NA	0 (0-0)	0 (0-0)	0 (0-0)	0 (0-0)
median	NA	1 (0-9)	<1 (0-<1)	<1 (0-<1)	<1 (0-<1)
mean	NA	15 (1-34)	9 (2-17)	2 (<1-5)	3 (<1--13)
95th percentile	NA	69 (5-100)	67 (12-97)	13 (2-29)	20 (<1-92)

Table 22. Grapes: Estimated Percent Mortality in Invertebrates Following Acute Exposure to ChemX
Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Daphnia	Shrimp
5th percentile	0 (0-0)	<1 (0-<1)
median	16 (<1-58)	97 (82-100)
mean	35 (16-51)	70 (57-80)
95th percentile	97 (83-100)	100 (100-100)

In the scenario for grapes in California, sensitive freshwater fish can be expected to experience significant mortality, with a best estimate of 15 % (1-34%). Five percent of the time, mortality would exceed 69% (5-100%). Invertebrates, similar to what is predicted for the other use scenarios, can be expected to suffer substantial mortalities, with sensitive species routinely experiencing very high levels of mortality 70% (57-80%), and 5% of the time experiencing total mortality of the exposed population.

2. Non-standard scenarios

a. Florida potatoes

Table 23. Florida Potatoes: Estimated Percent Mortality in Fish Following Acute Exposure to ChemX
Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Atlantic silverside	5th percentile species	Bluegill sunfish	Rainbow trout
5th percentile	36 (5-59)	5 (0-29)	<1 (0- <1)	<1 (0-1)
median	63 (50-76)	21 (<1-82)	2 (<1-8)	1 (<1-6)
mean	62 (50-74)	26 (1-74)	10 (2-29)	4 (<1-16)
95th percentile	84 (67-99)	63 (2 -100)	48 (8-100)	15 (<1-90)

Table 24. Florida Potatoes: Estimated Percent Mortality in Invertebrates Following Acute Exposure to ChemX
Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Daphnia	5th percentile species w/Daphnia 25th%tile	50th percentile species w/Daphnia 25th %tile	Shrimp
5th percentile	25 (0-73)	82 (<1-100)	5 (0-36)	92 (36-100)
median	74 (20-99)	99 (99-100)	23 (<1-73)	100 (100-100)
mean	68 (27-94)	96 (80-100)	30 (7-70)	98 (91-100)
95th percentile	95 (64-100)	100 (100-100)	75 (29-100)	100 (100-100)

In the scenario for potatoes grown in Florida, sensitive freshwater fish, unlike in Maine, can be expected to experience significant mortality in most exposure conditions, with mortalities expected to be in the range of 30% (1-74%). Infrequently, sensitive fish could experience approximately 60% mortality (2-100%). Again, very sensitive estuarine fish such as the Atlantic silverside will not tolerate exposure concentrations equivalent to those predicted to occur in farm ponds. Invertebrates, species such as Daphnia and those with similar sensitivities can be expected to incur 68% mortality (27-94%), with infrequent events (5% of the time) of extremely high average mortality (95%). Sensitive invertebrate species would routinely be expected to experience very high levels of mortality (average of 96%), with estuarine species such as shrimp incurring higher levels.

b. Iowa corn

As described above (section III. B.), Iowa was selected for use as a test case for examining model sensitivity to variation in selected model input parameters based on the high usage of

ChemX on corn in Iowa, based on BEAD data, and its availability as a standard corn scenario. To estimate the sensitivity of the predicted outcomes regarding mortality following acute exposures, specific exposure modeling parameters that were expected to have a substantial effect on exposure estimates, based on best professional judgement, were varied within individual PRZM/EXAMS simulations for Iowa corn. These parameters included pH of the receiving water body, soil aerobic metabolism rates, and the size of the treated field relative to the size of the water body receiving runoff from the field (see Table 10). Following the exposure analysis, it was decided to complete the effects analysis using a bounding-estimate approach. Thus, the Iowa corn scenarios providing the highest and lowest exposure estimates modeled were selected for effects analyses. The Iowa corn scenarios providing the highest exposure estimate was scenario 6 (pH 6.2, 90th% soil aerobic metabolism half-life, large field-to-pond size ratio). The lowest exposure estimate was found in scenario number 15 (pH 9, mean soil aerobic metabolism half-life, small field-to-pond size ratio.) All eight scenarios generated for a pH 7 pond were also subjected to further analyses.

Table 25. Iowa Corn Scenario 10 (pH 7, 90% aerobic metabolism, standard scenario) Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations.
Note: Best Fit to exposure data is marginal. EDF data below (in Table 26) provide superior estimation.

	Rainbow trout	Daphnia
5th percentile	<1 (0-1)	2 (<1-7)
median	<1 (0-1)	6 (1-18)
mean	<1 (0-1)	9 (1-24)
95th percentile	<1 (0-2)	24 (3-60)

Table 26. Iowa Corn Scenario 10 (pH 7, 90% aerobic metabolism, standard scenario): Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Empirical Model Simulations: Empirical Distribution for Exposure. 12.5 Million Simulations

	Rainbow trout	Daphnia
5th percentile	<1 (0-<1)	3 (<1-9)
median	<1 (0-<1)	5 (1-15)
mean	<1 (0-1)	10 (1-25)
95th percentile	<1 (0-2)	34 (4-77)

Table 27. Iowa Corn Scenario 7 (pH 7, 90% aerobic soil metabolism, small field:pond ratio) Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Rainbow trout	Daphnia
5th percentile	<1 (0- <1)	2 (<1-8)
median	<1 (<1- 2)	28 (4-66)
mean	1 (<1-4)	36 (12-61)
95th percentile	5 (<1-14)	91 (49-100)

Table 28. Iowa Corn Scenario 7 (pH 7, 90% aerobic soil metabolism, small field:pond ratio) Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Empirical Model Simulations: Empirical Distribution for Exposure. 12.5 Million Simulations

	Rainbow trout	Daphnia
5th percentile	<1 (0- <1)	3 (<1-9)
median	<1 (0- 1)	25 (2-71)
mean	1 (<1-3)	35 (11-60)
95th percentile	4 (<1-14)	89 (46-100)

Table 29. Iowa Corn Scenario 8 (pH 7, 90% aerobic soil metabolism, medium field:pond ratio) Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Rainbow trout	Daphnia
5th percentile	<1 (0- <1)	2 (<1-5)
median	<1 (<1-2)	35 (5-76)
mean	2 (<1-6)	41 (16-64)
95th percentile	10 (1-30)	95 (70-100)

Table 30. Iowa Corn Scenario 8 (pH 7, 90% aerobic soil metabolism, medium field:pond ratio) Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Empirical Model Simulations: Empirical Distribution for Exposure. 12.5 Million Simulations

	Rainbow trout	Daphnia
5th percentile	<1 (0- <1)	3 (<1-9)
median	<1 (0- 1)	33 (3-80)
mean	1 (<1-4)	40 (14-64)
95th percentile	6 (1-19)	93 (60-100)

Table 31. Iowa Corn Scenario 9 (pH 7, 90% aerobic soil metabolism, large field:pond ratio) Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Rainbow trout	Daphnia
5th percentile	<1 (0-1)	4 (<1-14)
median	1 (<1-4)	61 (15-98)
mean	7 (2-13)	57 (28-80)
95th percentile	39 (11-74)	99 (96-100)

Table 32. Iowa Corn Scenario 9 (pH 7, 90% aerobic soil metabolism, large field:pond ratio) Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Empirical Model Simulations: Empirical Distribution for Exposure. 12.5 Million Simulations

	Rainbow trout	Daphnia
5th percentile	<1 (0- <1)	3 (<1-10)
median	1 (0-5)	63 (15-99)
mean	5 (1-10)	58 (32-79)
95th percentile	23 (7-43)	98 (93-100)

Table 33. Iowa Corn Scenario 3 (pH 6.2, 90th percentile soil metabolism, large field:pond ratio) Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Theoretical Model Simulations: Fitted Distribution for Exposure. 1.25 Million Simulations

	Rainbow trout	Daphnia
5th percentile	<1 (<1-2)	46 (9-90)
median	5 (<1-15)	94 (70-100)
mean	10 (3-19)	87 (64-98)
95th percentile	36 (16-58)	99 (99-100)

Table 34. Iowa Corn Scenario 3 (pH 6.2, 90th percentile soil metabolism, large field:pond ratio) Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Empirical Model Simulations: Empirical Distribution for Exposure. 12.5 Million Simulations

	Rainbow trout	Daphnia
5th percentile	<1 (0-2)	38 (1-92)
median	5 (<1-15)	92 (55-100)
mean	10 (4-19)	84 (56-97)
95th percentile	33 (15-53.)	99 (96-100)

Iowa Corn Scenario 18 (pH 9, Mean soil metabolism, Small field:pond ratio)
Theoretical Model Simulations not done because best fit to exposure data was not an acceptable fit. See Empirical Fit data below.

Table 35. Iowa Corn Scenario 18 (pH 9, Mean soil metabolism, Small field:pond ratio) Estimated Percent Mortality in Fish and Invertebrates Following Acute Exposure to ChemX Empirical Model Simulations: Empirical Distribution for Exposure. 12.5 Million Simulations

	Rainbow trout	Daphnia
5th percentile	<1 (0- <1)	<1 (<1- <1)
median	<1 (0- <1)	1 (<1-7)
mean	1 (<1-2)	17 (6-31)
95th percentile	3 (<1-11)	84 (35-100)

Discussion of the effect on exposure estimates of the various factors (pH, aerobic metabolism, field:pond ratio) can be found section VI B. (sensitivity snalysis). In general, freshwater fish such as rainbow trout will be expected to experience less than 10% mortality following application of ChemX to corn in Iowa. However 5% of the time they could experience more than 30% mortality. This higher mortality rate was associated with larger fields than the standard EFED scenario. Invertebrates such as *D. magna* can be expected to experience modest to severe mortalities fairly routinely, depending on the conditions. The best estimate of *Daphnia* mortality associated with the standard scenario (pH 7 pond, and 10 acre field draining into a 1 acre pond), was 10% (1-25); 5% of the time the standard scenario would result in invertebrate mortality exceeding 34% (4-77%). By increasing the size of the field draining into the pond, the best estimate of *Daphnia* mortality increased to 35% for a small field, 40% for a medium field, and 58% for a large field. For all scenarios other than the low-estimating standard scenario, 5% of the time, nearly 100% of the local population would be expected to be killed (89-98%).

Overall, fish and invertebrate risk was found to be highest where the field:pond size ratio is large and/or pH of the water is acidic.

B. Chronic effects

Available chronic data were limited and, therefore, fewer scenarios were considered sufficient to cover the range of outcomes. An exceedence probability approach was taken to evaluate the potential chronic effects of ChemX usage on aquatic animal species. Exposure intervals evaluated were peak yearly maxima, 96 hour, 21 day, 60 day and 90 day yearly maxima of running averages. For illustrative purposes, only the peak and 60 day running averages are compared to fish NOECs (ENEC, for bluegill) and LOECs below, while only the peak and 21 day running averages are compared to invertebrate NOECs and LOECS, due to the relevance of these longer 60 and 21 day intervals to test durations for fish and invertebrates, respectively. It should be noted that predicted effects based on the comparison to longer duration exposure periods does not take into account potential delayed effects from short duration exposures, since the fish and invertebrate toxicity test designs do not take into account these types of latent effects.

Both maximum and typical, or average rate, depending on available usage data, were evaluated. Typical application rates were based on usage distribution data provided by BEAD for 1994-1995. Average application rates were based on information provided through consultation with BEAD, when usage distribution data was not available. Corn was modeled in Ohio, cotton in Mississippi, potatoes in Maine, and grapes were modeled with a California scenario. The values reported below are based on the commercial Monte Carlo software-fitted distributions. The results based on distributions derived via the *Expert Fit*™ software were not significantly different, and were limited to peak exposures for this analysis. Exceedence frequency graphs for the chronic data are given in the appendix.

The probability of exceeding a given chronic endpoint is listed in tables below.

1. Ohio Corn

a. Corn - Maximum Application Rate

Chronic effects were predicted in bluegill, based on the estimated no-effect concentration (ENEC) exposure at the maximum application rate for corn. Two applications at the maximum application rate of 1 lb ai/A were simulated.

Table 36. Percent Probability of Exceeding Chronic Endpoint Following ChemX Use on Corn at Maximum Application Rate (1 lb ai/A, 2 applications)

	Species and Chronic Endpoint				
Exposure Duration	Bluegill ENEC[1] (6 ppb)	Rainbow trout NOEC (25 ppb)	Rainbow trout LOEC (57 ppb)	*Daphnia* NOEC (10 ppb)	*Daphnia* LOEC (27 ppb)
Short[2]	100 %	7 %	0 %	100 %	3 %
Long [3]	100 %	1 %	0 %	99 %	< 1 %

[1] Bluegill ENEC: Estimated No-effect Concentration based on acute to chronic ratio determined for rainbow trout, applied to bluegill acute data to estimate no-effects concentration for bluegill (no chronic test data was available for bluegill).

[2] Short exposure duration was based on maximum annual peak concentrations from exposure modeling

[3] Long exposure duration varied between test species to reflect chronic test durations: 60 days was used as the long exposure duration for fish, 21 day was used for *Daphnia magna* (invertebrate). Long exposure duration data were based on annual maximum running averages from exposure model data.

Yearly maximum peak concentrations, and maxima of 96 hour, 21 day and 60 day running average concentrations all exceeded the bluegill ENEC. The bluegill ENEC was exceeded 100% of the time even for the 90 day time interval. The NOEC for Rainbow trout were exceeded less than 7 and 5% of the time for all peak and 96 hour exposures. The NOEC was exceeded 1% or less of the time for all longer time intervals. The LOEC was not exceeded for any time interval.

For invertebrates, chronic effects were predicted based on the NOEC and LOECs for *Daphnia magna*. For peak and 96 hour exposure intervals, the *Daphnia* NOEC was exceeded over 98% of the time for peak, 96 hour and 21 day intervals, and was exceeded 69% of the time for the 60-day interval. The LOEC was exceeded less than 5% of the time for all time periods.

b. Corn - Typical Application Rate

Table 37. Percent Probability of Exceeding Chronic Endpoint Following ChemX Use on Corn at the Typical Application Rate (0.75 lbs ai/A, 2 applications)

	Species and Chronic Endpoint				
Exposure Duration	Bluegill ENEC (6 ppb)	Rainbow trout NOEC (25 ppb)	Rainbow trout LOEC (57 ppb)	*Daphnia* NOEC (10 ppb)	*Daphnia* LOEC (27 ppb)
Short	100 %	< 1 %	<1 %	96 %	< 1 %
Long	97 %	< 1 %	<1 %	68 %	< 1 %

In an exceedence frequency analysis, potential chronic effects were predicted in bluegill, based on the estimated no-effect concentration (ENEC) exposure at the typical application rate of 0.75lbs ai/A for corn, with two applications per year. Yearly peaks, and maxima of 96 hour, 21 day running averages all exceeded the bluegill ENEC for every year modeled. For the 60 day and 90 day intervals, the bluegill ENEC was exceeded in 97% and 74% of the years, respectively.The NOEC and LOEC for Rainbow trout were exceeded less than 1% of the time for all time exposure intervals.

For peak and 96 hour exposure intervals, the *Daphnia* NOEC was exceeded 96 and 94% of the time, respectively. The LOEC was exceeded less than 1% of the time for the same time periods. For 21 day and 60 day time intervals, the NOEC was exceeded 68 of the time, while the LOEC was exceeded less than 1% of the time.

2. Mississippi Cotton
    a. Cotton- Maximum Application Rate

Table 38. Percent Probability of Exceeding Chronic Endpoint Following ChemX Use on Cotton at the Maximum Application Rate (1 lb ai/A)

	Species and Chronic Endpoint				
Exposure Duration	Bluegill ENEC[1]	Rainbow trout NOEC	Rainbow trout LOEC	*Daphnia* NOEC	*Daphnia* LOEC
Short[2]	49 %	4 %	<1 %	28 %	3 %
Long[3]	27 %	< 1 %	<1 %	21 %	1 %

[1] Bluegill ENEC: Estimated No-effect Concentration based on acute to chronic ratio determined for rainbow trout, applied to bluegill acute data to estimate no-effects concentration for bluegill (no chronic test data was available for bluegill).
[2] Short exposure duration was based on maximum annual peak concentrations from exposure modeling
[3] Long exposure duration varied between test species to reflect chronic test durations: 60 days was used as the long exposure duration for fish, 21 day was used for *Daphnia magna* (invertebrate). Long exposure duration data were based on annual maximum running averages from exposure modeling data.

After a single application to cotton at the maximum application rate, the probability of exceeding the bluegill ENEC for peak, 96 hour and 21 day interval was 40-50%. The probability of exceeding the ENEC was 27% for the 60 day time interval. The probability of exceeding the Rainbow trout NOEC or LOEC in a given year was less than 5% for all time periods examined.

The *Daphnia* NOEC was predicted to be exceeded 20 to 30% of the time, for the peak exposure, 96 hour and 21 day time periods. The LOEC was exceeded less than 5% of the time for all time intervals.

b. Cotton- Average Application Rate

Table 39. Percent Probability of Exceeding Chronic Endpoint Following ChemX Use on Cotton at the Average Application Rate (0.5 lb ai/A)

	Species and Chronic Endpoint				
Exposure Duration	Bluegill ENEC[1]	Rainbow trout NOEC	Rainbow trout LOEC	*Daphnia* NOEC	*Daphnia* LOEC
Short[2]	26 %	<1 %	0 %	10 %	<1 %
Long[3]	9 %	< 1 %	0 %	6 %	<1 %

3. Maine Potatoes

a. Potatoes- Maximum Application Rate

Table 40. Percent Probability of Exceeding Chronic Endpoint Following ChemX Use on Potatoes at the Maximum Application Rate (1 lb ai/A).

	Species and Chronic Endpoint				
Exposure Duration	Bluegill ENEC[1]	Rainbow trout NOEC	Rainbow trout LOEC	*Daphnia* NOEC	*Daphnia* LOEC
Short[2]	100 %	41 %	<1 %	100 %	25 %
Long[3]	100 %	< 1%	<1 %	100 %	8 %

[1] Bluegill ENEC: Estimated No-effect Concentration based on acute to chronic ratio determined for rainbow trout, applied to bluegill acute data to estimate no-effects concentration for bluegill (no chronic test data was available for bluegill).
2 Short exposure duration was based on maximum annual peak concentrations from exposure modeling
[3] Long exposure duration varied between test species to reflect chronic test durations: 60 days was used as the long exposure duration for fish, 21 day was used for *Daphnia magna* (invertebrate). Long exposure duration data were based on annual maximum running averages from exposure modeling data.

The bluegill ENEC was exceeded 100% of the time for all time intervals. The rainbow trout NOEC was exceeded 40-50% of the time for the peaks and 96 hour intervals, 15% of the time in the 21 day time period average, and less than 1 % of the time for the 60 day time period. The probability of exceeding the LOEC was less than 1% for all time intervals.

The probability of exceeding the Daphnia LOEC was 100% for the peak, 96 hour and 21 day intervals. The probability of exceeding the LOEC was 25%, for the peak and 96 hour periods, and 8% for the 21 day period.

b. Potatoes- Average Application Rate

Table 41. Percent Probability of Exceeding Chronic Endpoint Following ChemX Use on Potatoes at the Average Application Rate (0.8 lbs ai/A) .

	Species and Chronic Endpoint				
Exposure Duration	Bluegill ENEC[1]	Rainbow trout NOEC	Rainbow trout LOEC	*Daphnia* NOEC	*Daphnia* LOEC
Short[2]	100 %	14 %	0 %	100 %	7 %
Long [3]	100 %	<1 %	0 %	100 %	< 1 %

At the average application rate of 0.8 lbs ai/A, the bluegill ENEC was exceeded 100% of the time for all time intervals. The Rainbow trout LOEC was exceeded approximately 10% of the time for the peak and 96 hour periods, and 2% of the time for the 21 day interval, and less than 1% of the time for the 60 day interval. The LOEC was never exceeded.

The *Daphnia* NOEC was exceeded 100% of the time for peak, 96 hour and 21 day intervals. The LOEC was exceeded less than 10% of the time for the same intervals.

4. California Grapes

a. Grapes- Maximum Application Rate

Table 42. Percent Probability of Exceeding Chronic Endpoint Following ChemX Use on Grapes at the Maximum Application Rate (10 lbs ai/A, 1 application) .

	Species and Chronic Endpoint				
Exposure Duration	Bluegill ENEC[1]	Rainbow trout NOEC	Rainbow trout LOEC	*Daphnia* NOEC	*Daphnia* LOEC
Short[2]	75 %	47 %	26 %	66 %	45 %
Long [3]	64 %	31 %	9 %	61 %	40 %

After a single maximum application of 10 lbs ai /A, the bluegill ENEC was exceeded 70% of the time for peak, 96 hour and 21day intervals, and 64% of the time at the 60 day interval. The rainbow trout NOEC was exceeded 40-50% of the time for peak, 96 hour and 21 day intervals, and 31% of the time for the 60 day interval. The LOEC was exceeded 20-26% of the time for the peak to 21 day intervals, and 9% of the time for the 60 day interval.

The *Daphnia* NOEC was exceeded more than 60% of the time for the peak, 96 hour and 21 day periods. The LOEC was exceeded 40% or more of the time for the same intervals.

b. Grapes - Average Application Rate

Table 43. Percent Probability of Exceeding Chronic Endpoint Following ChemX Use on Grapes at the Average Application Rate (3 lbs ai/A, 1 application) .

	Species and Chronic Endpoint				
Exposure Duration	Bluegill ENEC[1] (5.7 ppb)	Rainbow trout NOEC (24.8 ppb)	Rainbow trout LOEC (56.7 ppb)	*Daphnia* NOEC (9.8 ppb)	*Daphnia* LOEC (27.0 ppb)
Short[2]	54 %	16 %	<1 %	41 %	14 %
Long [3]	37 %	2 %	<1 %	34 %	8 %

The bluegill ENEC was exceeded 32-54% of the time for all intervals after a single average application of 3 lbs ai/A. The rainbow trout NOEC was exceeded 10-16% of the time for peak, 96 hour and 21 day time periods, and 2% of the time for the 60 day interval. The LOEC was exceeded less than 1% of the time for all intervals.

For the peak, 96 hour and 21 day intervals the Daphnia NOEC was exceeded 34-40% of the time, while the LOEC was exceeded 8-14% of the time.

VI. Sensitivity Analyses

Sensitivity analyses were conducted for the ChemX risk assessment. As noted in the Agency's Guiding Principles to Monte Carlo Analyses (1997) "sensitivity analysis attempts to provide a ranking of the model's input assumptions with respect to their contribution to model output variability or uncertainty."

Three sensitivity analyses were performed; (1) an analysis of the sensitivity of the commercial Monte Carlo software-based model to the 4 parameters in the model, (2) an analysis of the sensitivity of the predicted outcomes to the use of best-fit exposure distributions versus empirical fits, and (3) an analysis of the effect of varying selected PRZM/EXAMS input parameters, based on best professional judgement of likely significant input parameters.

A. Sensitivity Analysis of Input Parameters for Commercial Monte Carlo Software-Based Model

An analysis of the sensitivity of the model around the central tendency estimates of mortalities was performed, via the sensitivity analysis option within the commercial Monte Carlo software used. Analyses were conducted for several species, including selected fish and invertebrate species, for 3 crops: corn, cotton and potatoes. Analyses were conducted both with the correlations between the parameters used in the analysis, and with them not included. The tables below show the sensitivity analyses based on rank correlation. Rank order analyses were conducted because of non-linearity within the data evaluated; i.e. some of the distribution were skewed. Ranking of the model's sensitivity to the input parameters, when the correlation between parameters is included in the analyses, are given on left side of each cell. Correlation coefficients given in parentheses. Sensitivity values produced when correlations were turned off are on the right side of each cell.

Table 44. Sensitivity Analysis Based for Ohio Corn on Rank Correlation: Fish Mortality Following ChemX Application. Ranking of the model's sensitivity to the input parameters, when the correlation between parameters is included in the analyses, are given on left side of each cell. Correlation coefficients given in parentheses. Sensitivity values produced when correlations were turned off are on the right side of each cell.

	5th Percentile Fish		Silverside	
	Correlations On Rank (r)	Correlations Off Rank (r)	Correlations On Rank (r)	Correlations Off Rank (r)
Slope	1 (0.94)	1 (0.94)	4 (-0.05)	2 (0.63)
Intercept	2 (-0.93)	2 (0.07)	1 (0.24)	1 (0.68)
Scale	3 (0.05)	3 (0.02)	2 (0.10)	3 (0.02)
Shape	4 (-0.03)	4 (-0.01)	3 (-0.06)	4 (-0.01)

Table 45. Sensitivity Analysis for Ohio Corn. Based on Rank Correlation: Invertebrate Mortality Following ChemX Application.

	5^{th} Percentile Invertebrate		*Daphnia magna*	
	Correlations On Rank (r)	Correlations Off Rank (r)	Correlations On Rank (r)	Correlations Off Rank (r)
Slope	2 (-0.82)	1 (0.45)	1 (0.65)	1 (0.78)
Intercept	1 (0.89)	2 (0.85)	2 (-0.57)	2 (0.53)
Scale	3 (-0.04)	3 (-0.01)	3 (0.09)	3 (0.02)
Shape	4 (0.01)	3 (0.01)	4 (-0.05)	4 (-0.01)

Table 46. Sensitivity Analysis for MS Cotton Based on Rank Correlation: Fish and Invertebrate Mortality Following ChemX Application

	Silverside		5^{th} Percentile Invertebrate	
	Correlations On Rank (r)	Correlations Off Rank (r)	Correlations On Rank (r)	Correlations Off Rank (r)
Slope	2 (-0.18)	2 (0.28)	2 (-0.55)	2 (0.25)
Intercept	1 (0.22)	1 (0.46)	1 (0.58)	1 (0.70)
Scale	3 (0.15)	3 (0.13)	3 (0.10)	3 (0.10)
Shape	4 (0.11)	4 (0.08)	4 (0.06)	4 (0.04)

Table 47. Sensitivity Analysis Based for Maine Potatoes Based on Rank Correlation: Fish Mortality Following ChemX Application.

	5th Percentile Fish	
	Correlations On Rank (r)	Correlations Off Rank (r)
Slope	1 (0.96)	1 (0.96)
Intercept	2 (-0.94)	2 (0.07)
Scale	3 (0.04)	3 (0.03)
Shape	4 (-0.01)	4 (-0.02)

Table 48. Sensitivity Analysis for Maine Potatoes. Based on Rank Correlation: Invertebrate Mortality Following ChemX Application.

	5th Percentile Invertebrate		*Daphnia magna*	
	Correlations On Rank (r)	Correlations Off Rank (r)	Correlations On Rank (r)	Correlations Off Rank (r)
Slope	2 (-0.78)	1 (0.49)	1 (0.80)	1 (0.81)
Intercept	1 (0.87)	2 (0.83)	2 (-0.71)	2 (0.49)
Scale	3 (0.01)	3 (0.04)	3 (0.06)	3 (0.04)
Shape	3 (-0.01)	4 (-0.01)	4 (-0.01)	4 (0.02)

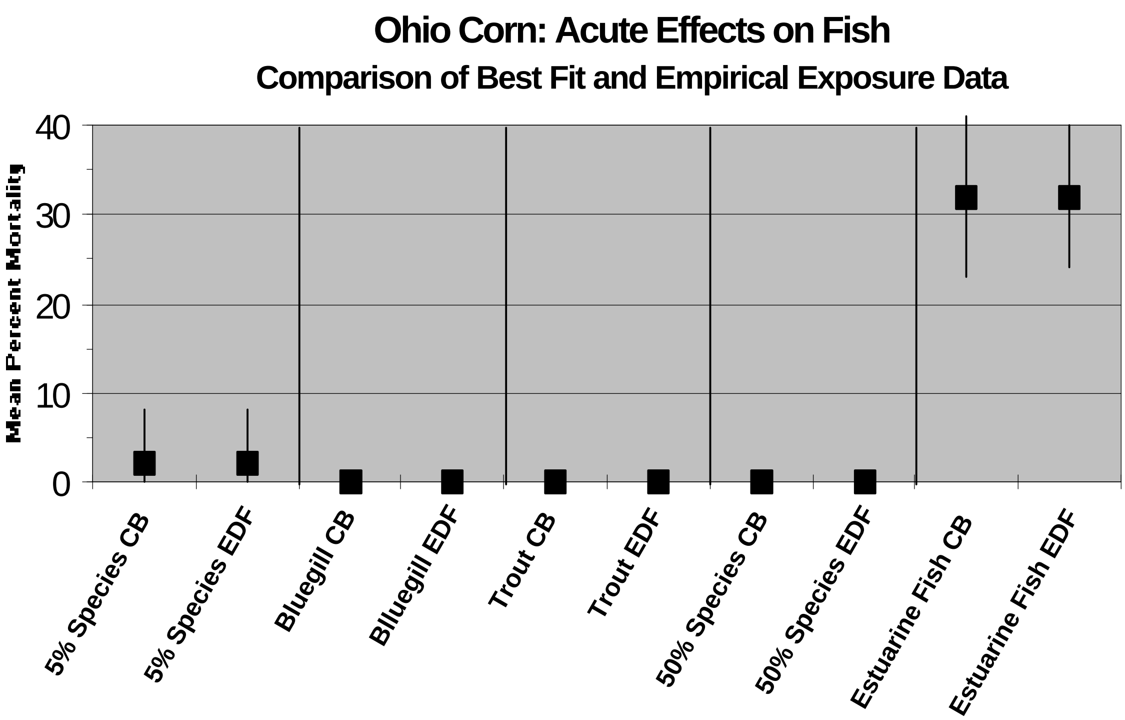
It is difficult to make a conclusive statement regarding the sensitivity of the model because of the nature of the uncertainty. Because for some species the dose-response curve was often completely above or below the exposure data, it is difficult to generalize across species. However, the standard errors associated with the species toxicity curves appeared to be driving the sensitivity analyses: the data indicate that in nearly all cases, the Monte Carlo risk assessment model was most sensitive to uncertainties in the effects parameters, the slope and intercept of the acute toxicity curve, within each given crop/scenario. It should be noted that the slope and intercept of the dose-response curves were closely correlated, and thus the ranking of those two parameters should be considered equivalent. The estimated uncertainties for effects and exposure were based only on the probit analyses of the toxicity data and the PRZM/EXAMS model estimates of the exposure, respectively. As noted above, both the uncertainty in the expected toxicity in the field and the uncertainty in the expected exposure concentrations actually occurring in the environment are not represented in this analysis. However, this analysis does indicate what parameters are contributing most to uncertainty within the current Tier 2 refined screen: the effects data.

B. Comparison of Two Models for Risk Analysis: Sensitivity of the Predictions to Exposure Distribution Selection

A comparison of the analyses based on the commercial Monte Carlo software, using a theoretical exposure distribution, and the EPA-authored C-Program, using an empirical exposure distribution was performed. The purpose of the comparison was to evaluate the effect of applying a fitted distribution to the exposure data in the analyses, versus using the empirical distribution of the exposure model data, in the C program. The two models were also compared for speed and ease of use in future probabilistic assessments. In general the approaches yielded very similar risk estimates, except in some cases in the tails of the risk predictions. Deviations in the tails between the two models, may have been due to differences in the exposure data at the tails, including the lack of an upper bound on the theoretical distributions fitted to the exposure data which were used in conjunction with the commercial Monte Carlo software, as described above. The difference could also have been due, in part, to a more complete characterization of the predicted outcomes in the tails of the distributions in the empirically-based C program, as a result of the superior computational analysis available through the use of C. That is, the commercial Monte Carlo limits the second dimension of the Monte Carlo analysis to 250 simulations, whereas 2500-5000 outer loop simulations were performed with the C program. Because the predictions in the tails of the risk distribution were similar for all fitted and empirical scenarios except for the Mississippi cotton scenario, it appears that in most cases the additional simulations available through the use of the C program did not make a significant difference in the risk predictions, and that the differences in the Mississippi scenario were most likely due to the specifics of that particular fit for the exposure peaks, combined with the lack of an upper bound on the exposure estimates with the theoretical distribution used in the commercial Monte Carlo software analyses. The technical results were generally similar for the best estimates of mortality (mean estimates).

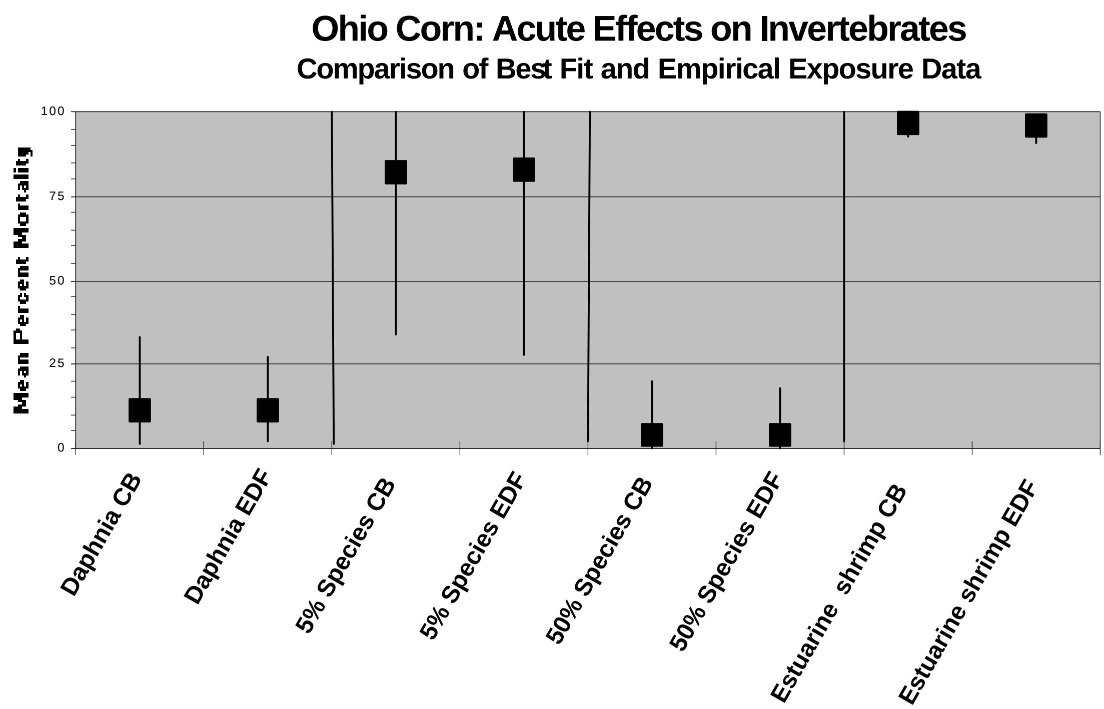
The theoretical program and empirical program approach both appear to be useful and valid, and not largely different in outcome. The theoretical program approach had two advantages, the ease of use and the automatic graphic production. The difference in ease of use with the commercial Monte Carlo program was somewhat offset by the lengthy simulation time. The running time for the commercial Monte Carlo program was over 20 minutes each, while the EPA C-based program took approximately 1 minute, even with its additional iterations. The rapid analysis with the EPA C-based program was useful in conducting a large number of runs, but if graphical output was needed, at this time, it would have to be manually produced through a graphing package used external to the analysis. The following six figures present these results for mean estimates in graphical form.

Figure 3. Graphical Comparison of Best-Fit versus Empirical Exposure Distributions Selection-Effects on Fish Mortality Predictions: Ohio Corn



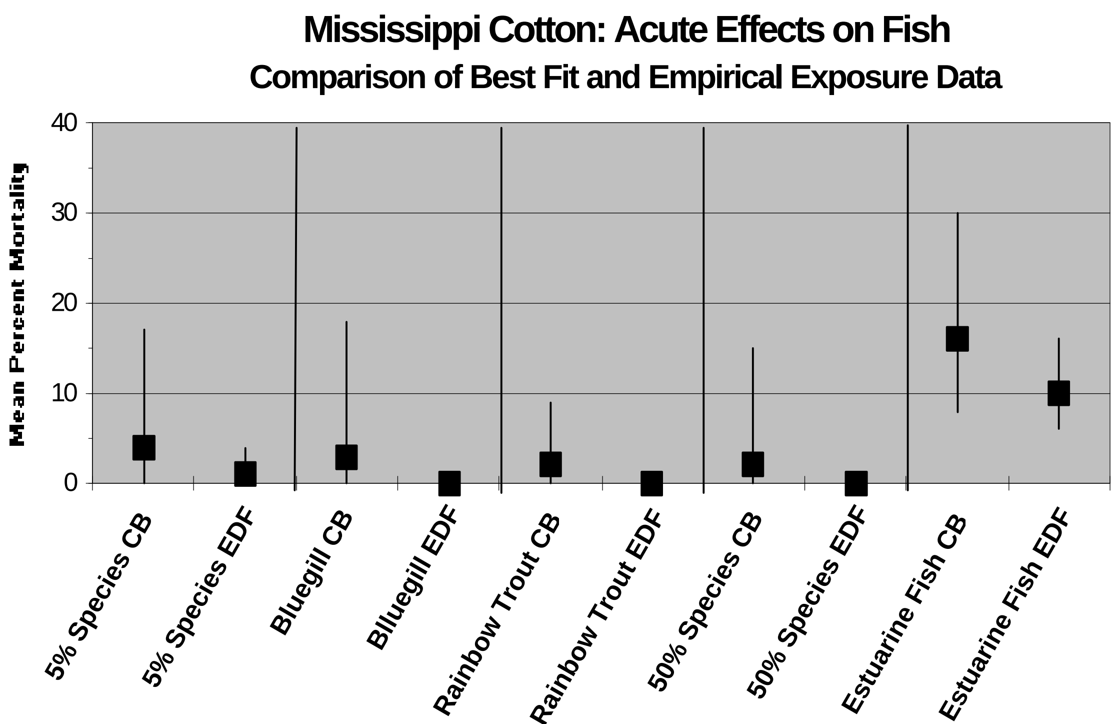
CB signifies use of Crystal Ball Software in combination with best-fit exposure distribution
EDF signifies use of Empirical Distribution Function for exposure data as described in text
Bars Indicate 5 and 95% confidence limits on the mean

Figure 4. Graphical Comparison of Best-Fit versus Empirical Exposure Distributions Selection-Effects on Invertebrate Mortality Predictions: Ohio Corn



CB signifies use of Crystal Ball Software in combination with best-fit exposure distribution
EDF signifies use of Empirical Distribution Function for exposure data as described in text
Bars indicate 5 and 95% confidence limits on the mean

Figure 5. Graphical Comparison of Best-Fit versus Empirical Exposure Distributions Selection-Effects on Fish Mortality Predictions: Mississippi Cotton



CB signifies use of Crystal Ball Software in combination with best-fit exposure distribution
EDF signifies use of Empirical Distribution Function for exposure data as described in text
Bars indicate 5 and 95% confidence limits on the mean

Figure 6. Graphical Comparison of Best-Fit versus Empirical Exposure Distributions Selection-Effects on Invertebrate Mortality Predictions: Mississippi Cotton

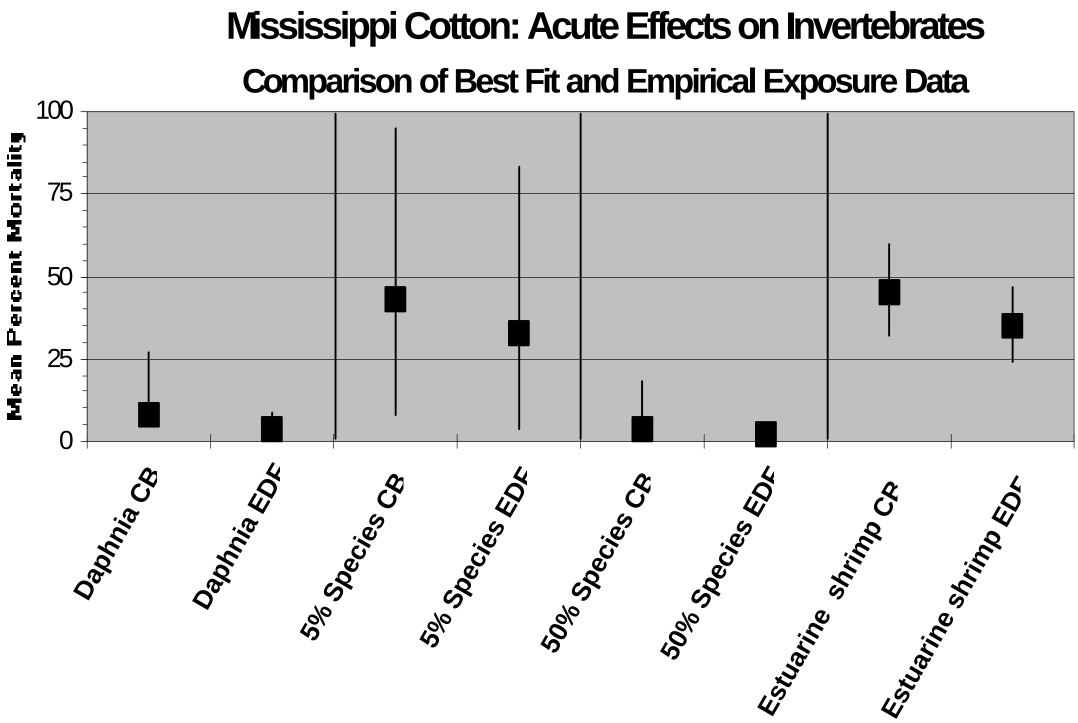


Figure 7. Graphical Comparison of Best-Fit versus Empirical Exposure Distributions Selection-Effects on Fish Mortality Predictions: Iowa Corn

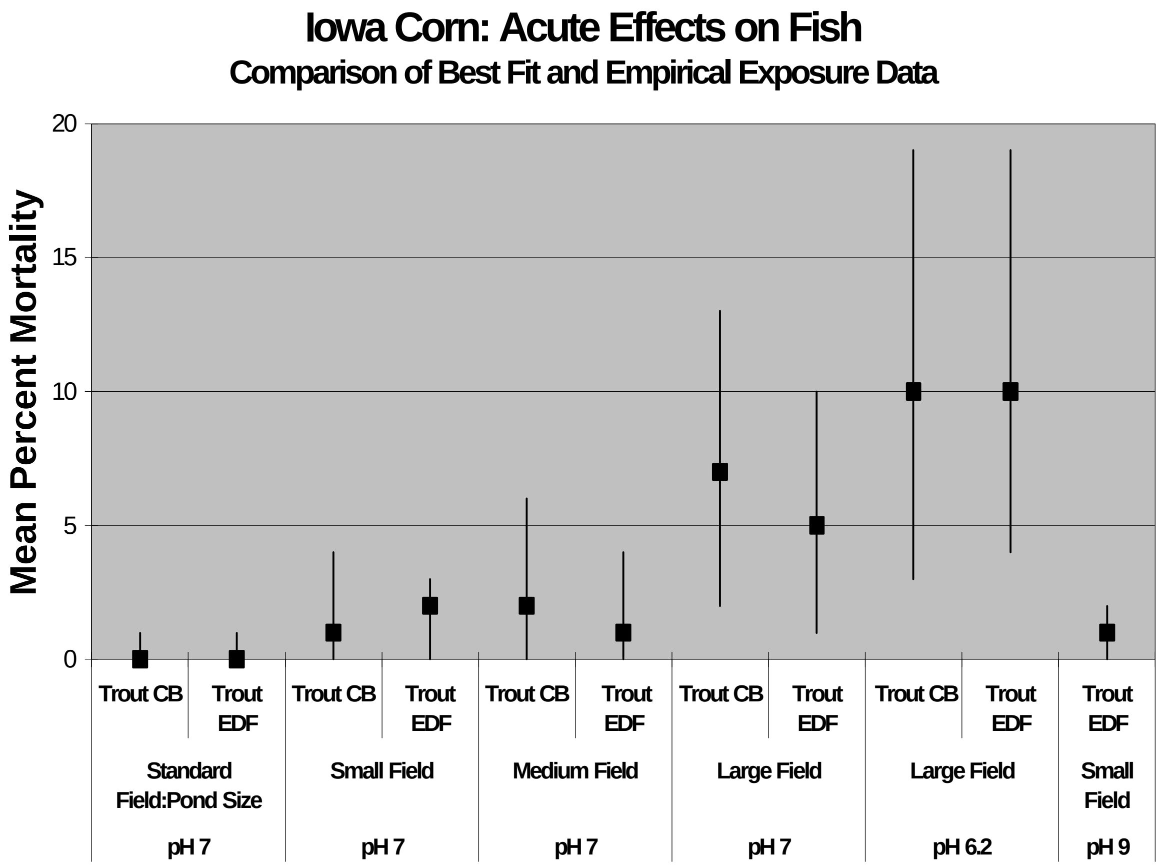
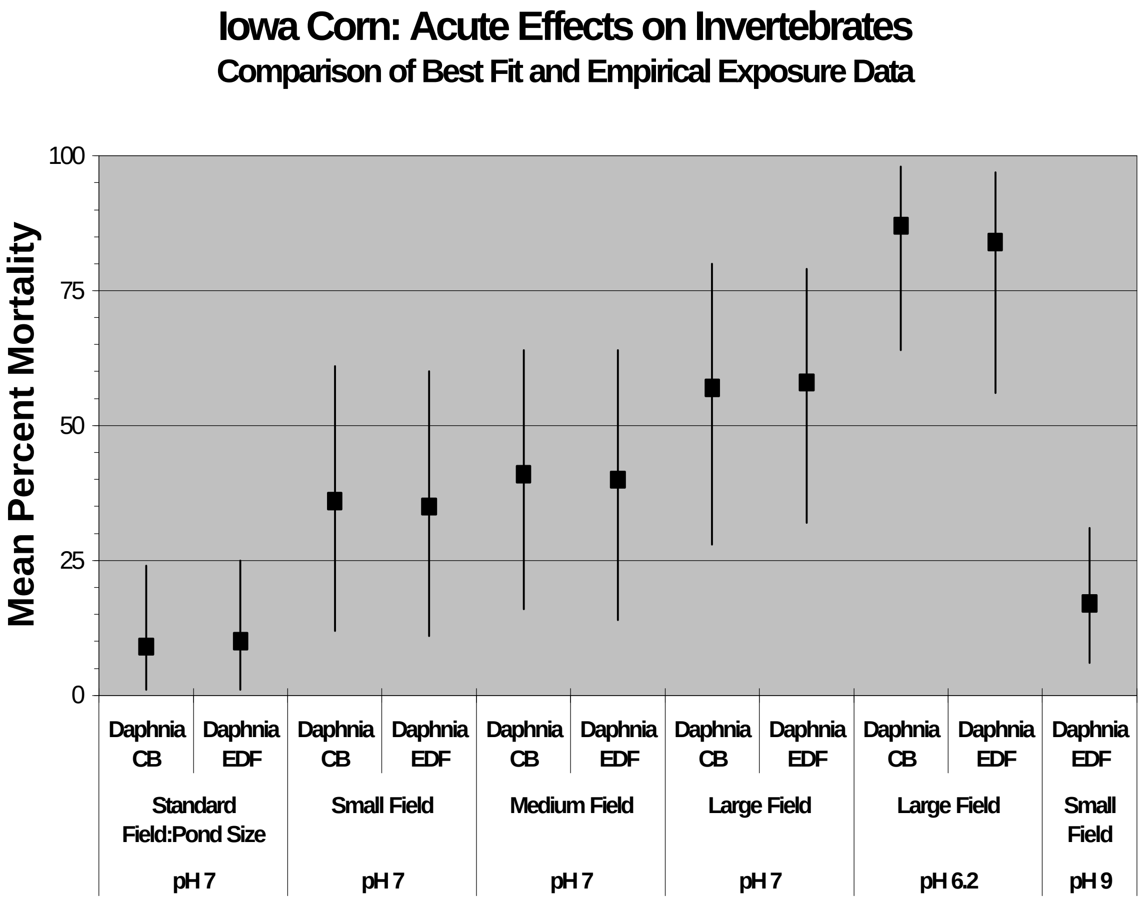


Figure 8. Graphical Comparison of Best-Fit versus Empirical Exposure Distributions Selection-Effects on Invertebrate Mortality Predictions: Iowa Corn



C. Results of the Exposure Modeling Sensitivity Analysis for Peak Concentrations: Evaluation of Sensitivity of the Model to Selected PRZM/EXAMS Input Parameters

The effect of varying PRZM/EXAMS scenario parameters was analyzed for impact on: (1) exposure estimates and, (2) effects risk estimates. The results are described in the following 2 sections.

1. Exposure results: Exposure Modeling Sensitivity Analysis

To estimate the sensitivity of the predicted outcomes regarding mortality following acute exposures, specific exposure modeling parameters that were expected to have a substantial effect on exposures estimates, based on best professional judgement, were varied within individual PRZM/EXAMS simulations. These parameters included pH of the receiving water body, soil aerobic metabolism rates, and the size of the treated field relative to the size of the water body receiving runoff from the field.

Using the 90th percentile of the soil aerobic metabolism half-lives (longer) instead of the mean half-life only increased the mean peak concentration by less than 1 percent for all modeled Iowa scenarios. The soil aerobic metabolism parameter varied in the scenario made no significant difference in the exposure estimates.

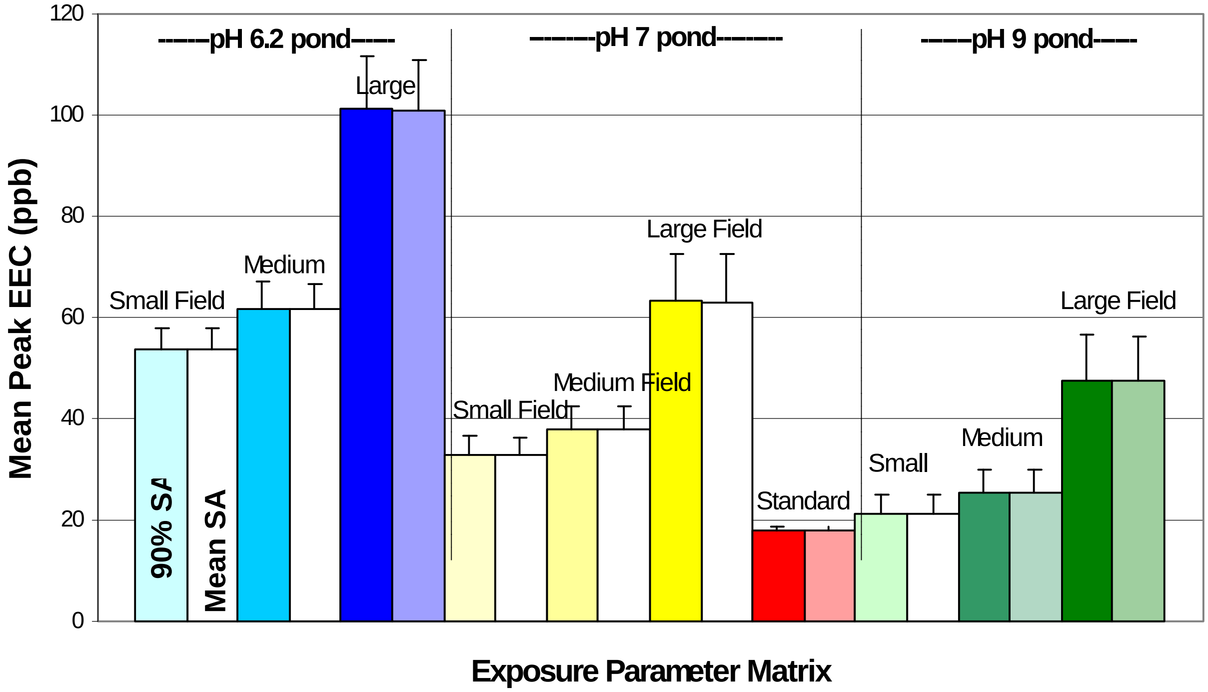
Decreasing the pH from the standard 7 to 6.2 increased the mean peak concentration by 1.6 fold (60%), while increasing the pH from the standard 7 to 9 decreased the mean peak concentration by 25-35%. Decreasing the pH from the 9 to 6.2 approximately doubled the mean peak concentration.

Increasing the field to pond size ratio from the standard scenario of 10:1 to the lowest field to pond ratio recommended for Iowa (48:1) nearly doubled the mean peak EEC, at a given pH (7), and increasing the field to pond ratio from the standard to the average field to pond ratio recommended for Iowa (60:1) doubled the mean peak EEC at pH 7. Increasing the field to pond ratio from the standard scenario to the maximum field to pond ratio recommended for Iowa (120:1) increased the mean peak concentration 3.5-fold, at a given pH (7). Increasing the field to pond ratio from the smallest to the largest recommended for Iowa increased the peak concentration approximately 2-fold at pH 7.

Given these results, it is concluded that for this set of analyses for ChemX use in Iowa, increasing the pH to 9 or decreasing the pH to 6, from the standard scenario's pond pH of 7, had somewhat less of an effect on peak EEC than changing the field: pond size ratio within the recommended range. Inter-scenario field to pond size ratio variability may have a more significant impact on EEC than inter-pond pH variability for ChemX.

The figure attached below depicts the exposure modeling sensitivity analysis. The bars represent standard errors.

Figure 9. Exposure Modeling Sensitivity Analysis for Iowa Corn.



90% SA denotes the use of the 90th percentile of the distribution of soil aerobic metabolism rates. Mean SA denotes the use of the mean soil aerobic metabolism rate.

2. Acute Effects Results: Exposure Modeling Sensitivity Analysis

Increasing the field size over that in the standard model did not have a large effect on mean mortality estimates for fish following peak exposure; both estimates were in the range of 10% mortality. Specifically, mean mortality estimates increased from less than 1% (5 and 95% confidence limits of 0 and 2%) in the standard pond scenario, to 7% (2-13%) by increasing the field to pond size ratio to the maximum recommended by the USDA for Iowa. A larger effect on invertebrate mortality estimates was observed when increasing field size. Mean mortality in invertebrates increased by 48%, from less than less than 9% (1-24%) in the standard pond scenario, to 57% (28-80%) in the maximum field:pond size scenario recommended by the USDA for Iowa. The difference between effects in fish and invertebrates observed when increasing field size was most likely due to a combination of the steeper dose-response slope associated with the invertebrate species modeled, over that of the fish, as well as the fact that the exposure peaks were falling within the range of significant invertebrate mortality levels, but were below that of the fish.

The effect of varying pH on fish mortality estimates was small, while, again, the effect on invertebrate mortality estimates was greater. Changing the pond pH from 7 to 6.2 only increased the mean mortality in fish by 3%, from 7% to 10% (3-19). Both of these scenarios were for a large field: pond size ratio. Increasing the pH to 9, while keeping the field:pond size the same, decreased the mean mortality to 1% (<1-2). Changing the pond pH from 7 to 6.2 increased the mean mortality in invertebrates by 30%, from 57% (28-80%) to 87% (64-98%). Both of these scenarios were, again, for a large field: pond size ratio. Increasing the pH to 9, while keeping the field:pond size the same, decreased the mean mortality by 40%, to 17% (6-31%).

As expected by the exposure estimates, varying the field size had a somewhat larger effect on mortality estimates than varying the pH, within the ranges examined. The graphs below show the differences in acute risk predictions for fish and invertebrates based on varying the selected model input parameters (*NB*: Scale differences for fish and invertebrate mortality).

Figure 10. Effect of Varying Selected PRZM/EXAMS Input Parameters on Mean Mortality Estimates for Fish

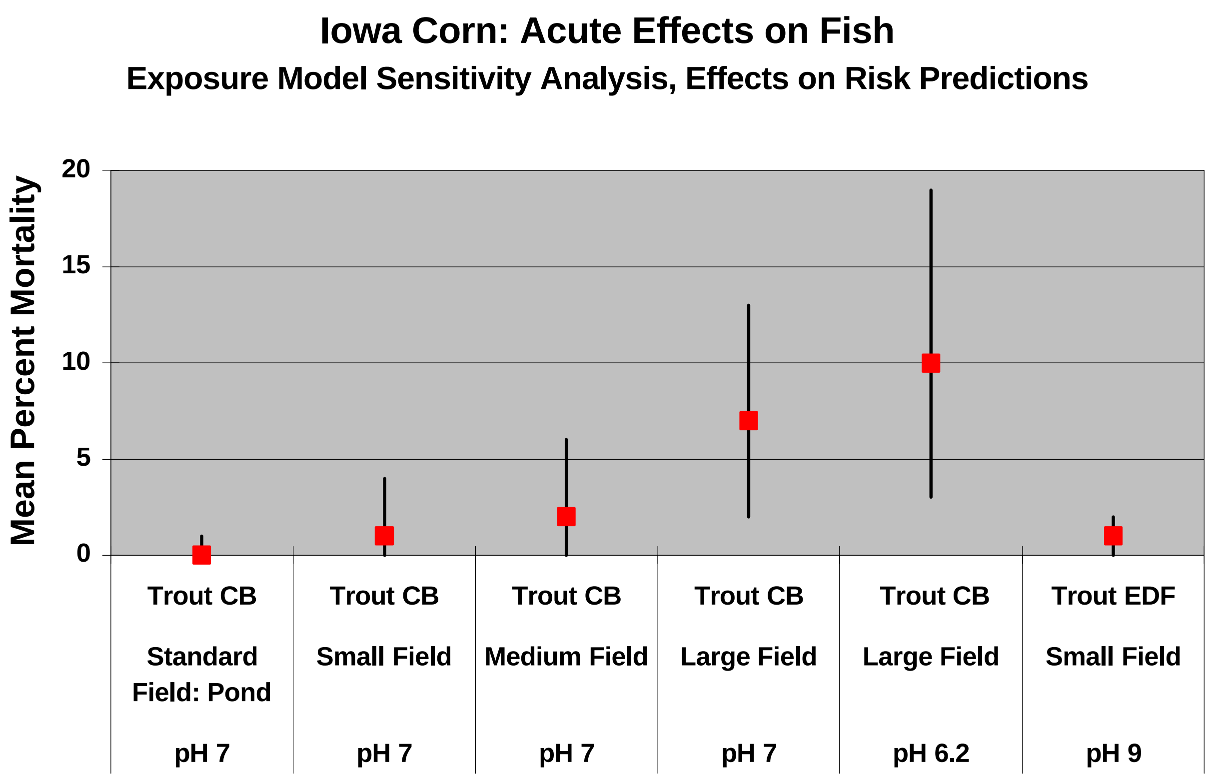
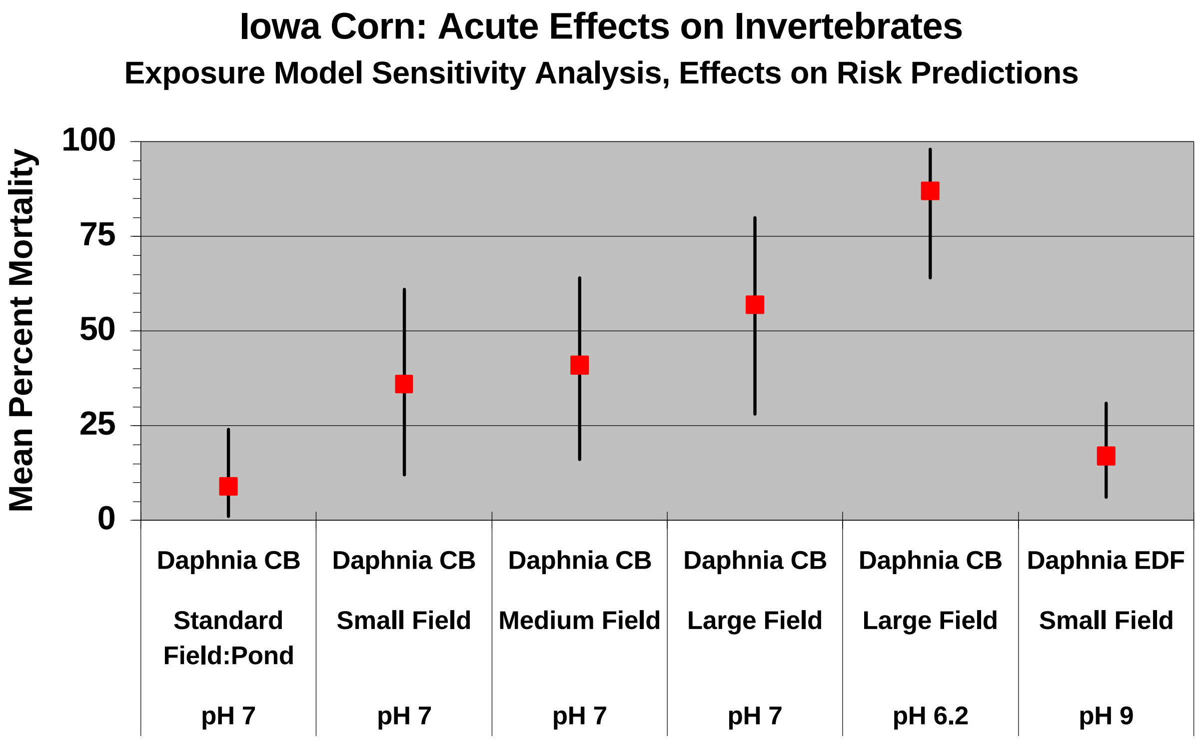


Figure 11. Effect of Varying Selected PRZM/EXAMS Input Parameters on Mean Mortality Estimates for Invertebrates



VII. Discussion

It is clear from the results of the ChemX deterministic risk assessment that further evaluation was warranted. This case study presented a refined risk assessment for selected ChemX uses, following the approaches outlined in EFED's implementation plan for conducting probabilistic aquatic organism risk assessments (US EPA, 2000).

On the basis of (1) application rates, (2) estimated exposure concentrations, (3) acreage treated, and (4) representativeness of the use site, the aquatic risk assessment focused on applications to corn, cotton, potatoes, and grapes. Standard scenarios evaluated in the deterministic risk assessment, including Ohio corn, Mississippi cotton, Maine potatoes, and California grapes were analyzed via probabilistic methods. The effect of varying specific parameters expected to have a large impact on exposure estimates (pond pH, field size, aerobic metabolism rates) was also examined through the Iowa corn scenario. Additional analyses included the comparison of two computer programs for Monte Carlo probabilistic risk analysis.

Acute analyses described the probability and magnitude of expected mortality. Chronic analyses, due to data and resource limitations, addressed only the probability of exceeding chronic risk assessment endpoints, and therefore could not predict the magnitude of potential chronic effects.

Based on RQs, the deterministic assessment concluded qualitatively that ChemX can pose a "high risk" to aquatic organisms. Based on probabilistic analyses, the use of ChemX can be expected to infrequently (5% of the time) result in significant freshwater fish mortalities and may routinely result in reduced growth and other chronic effects in exposed fish. Substantial mortalities and chronic effects to sensitive aquatic invertebrates may be expected to routinely occur after peak exposures. Estuarine fish and invertebrates, which are more sensitive than their freshwater relatives, are likely to experience substantial mortality when exposed to concentrations in their habitat equivalent to what has been modeled for farm ponds in the use scenarios studied.

Corn is the largest use crop for ChemX, with up to 2 million acres treated each year. For freshwater fish, mortality is expected to be less than 10% in virtually all cases, for even the most sensitive species associated with use on corn. However, use of ChemX at maximum rates on corn is predicted to provide exposures which will result in 75% mortality to the most sensitive invertebrates 95% of the time. For *Daphnia magna*, 11% mortality, on average, is estimated, with 40% or greater mortality occurring 5% of the time. Estuarine fish and invertebrates may be subject to much more risk. The best estimate of estuarine fish mortality is 32%, and over 96% mortality is expected for estuarine invertebrates. Chronic estimated no-adverse-effect-concentrations for fish, based on bluegill, are exceeded 99% of the time, even when a time-weighted average of up to 90 days is used. Invertebrates NOECs are exceeded nearly 100% of the time, even when a time-weighted average of up to 21 days is used for the standard Ohio corn scenario.

The use scenario for potatoes in Florida provide the greatest predicted aquatic risk. Sensitive freshwater fish (5^{th} percentile) are predicted to experience 26% mortality, on average, and more than 63% mortality 5% of the time. *D. magna* on average is expected to incur 68% mortality, with 95% or greater mortality occurring 5% of the time. Estuarine fish and invertebrates, if experiencing equivalent exposures in their habitat predicted for farm ponds, will experience very high mortality. The best estimate for estuarine fish mortality was 62%, with more than 84% mortality occurring 5% of the time. For estuarine invertebrates mortality was predicted to be nearly 100%.

The use on grapes in California provided risks similar to Florida potatoes. Sensitive freshwater fish (5^{th} percentile) are predicted to experience 15% mortality, on average, and more than 69% mortality 5% of the time. *D. magna* on average is expected to incur 35% mortality, with 97% mortality occurring 5% of the time. The risks for these species during infrequent events were higher for California grapes than for Florida potatoes, perhaps due to more frequent high exposure events in the grape scenario than in the modeled potato scenario. Estuarine fish and invertebrates, if experiencing exposures in their habitat equivalent to those predicted for farm ponds, would experience very high mortality.

Literature studies indicate that sublethal effects on fish from acute exposures to ChemX can be expected due to its chemical class and mode of action. These endpoints are generally not assessed by the standard toxicity test protocols used by EFED, and so are not included in this probabilistic refinement. Sublethal effects could be critical for endangered species.

The probability of high mortality rates for invertebrates will be likely to have an indirect effect on fish, as will the high probability of exceeding invertebrate chronic no-effects levels. Indirect effects on fish may include reduced juvenile fish survival due to reduced invertebrate food resources, with concomitant potential alterations in fish population structure, and potential decreased fish populations in use areas.

The effect of altering the exposure model scenario from the standard approach was examined for impacts on peak exposure concentration estimates and on expected mortality after peak exposures. For this Iowa corn scenario analysis for ChemX, there was not a significant difference in <u>exposure concentration</u> estimates using a mean soil aerobic metabolism rate or 90^{th} percentile value. Increasing the pH to 9 or decreasing the pH to 6, from the standard scenario's pond pH of 7, had less of an effect on peak concentration than changing the field: pond size ratio within the range recommended by the USDA for pond construction. Inter-scenario field to pond size ratio variability may have a more significant impact on peak EEC than inter-pond pH variability for ChemX.

Increasing the field size over that in the standard model did not have a large effect on <u>mean mortality estimates</u> for fish following peak exposure; both estimates were in the range of 10% mortality. A larger effect on invertebrate mortality estimates was observed when increasing field size. The difference between effects in fish and invertebrates observed when increasing field size was most likely due to a combination of the somewhat steeper dose-response slope associated with the invertebrate species modeled, over that of the fish species modeled (except bluegill), as well as the fact that the exposure peaks were falling within the range of significant invertebrate mortality levels, but were generally below that of the fish. The effect of varying pH on fish mortality estimates was small, while, again, the effect on invertebrate mortality estimates was greater. As expected by the exposure estimates, varying the field size had a marginally larger effect on mortality estimates than varying the pH, within the ranges examined.

A comparison of commercial Monte Carlo program and the EPA C program simulations was performed. The purpose of the comparison was to evaluate the effect of applying a fitted distribution to the exposure data in the commercial Monte Carlo program analyses, versus using the empirical distribution of the exposure model data in the C program. The two models were also compared for speed and ease of use in future probabilistic assessments. In general the approaches yielded very similar risk estimates, except in some cases in the tails of the risk predictions. The commercial Monte Carlo program had two advantages: its ease of use and automatic graphic production. The difference in ease of use with commercial Monte Carlo program was somewhat offset by the lengthy simulation time. The running time for the commercial Monte Carlo program simulations was over 20 minutes each, while the EPA C-based program took approximately 1 minute for more iterations. The rapid analysis with the EPA C program was useful in conducting a large number of runs, but if graphical output was needed, it would have to be manually produced through a graphing package used external to the analysis.

There are a number of uncertainties associated with both the refined and deterministic risk assessments that are not included in the ChemX risk assessment. These include uncertainty regarding the error introduced when extrapolating from laboratory to field effects at a given concentration. For example, mortality in the field could be greater in populations previously stressed by other pesticide exposures, temperature conditions, habitat loss, predation, or competition for limited resources, among other things. Overall field mortality could be lower if the laboratory population represented an unusually sensitive species. There is uncertainty associated with the use of single laboratory toxicity tests for a species. The experimental uncertainty regarding the representativeness of the test results could be reduced through replication of the toxicity tests for each species. There is uncertainty regarding the extrapolation of expected effects to more sensitive species, and the frequency with which these more sensitive species occur in ChemX use areas. There is uncertainty regarding the extrapolation to all invertebrates from a data set containing only arthropods. There is also uncertainty regarding the representativeness of the fate input parameters used in the exposure modeling; some input parameters were based on limited physico-chemical data. Another source of uncertainty is the use of exposure model-derived estimated concentrations to represent actual environmental concentrations. These uncertainties could be reduced through additional laboratory and field tests.

The uncertainties that were addressed in the probabilistic analyses, and which are included in the bounds given for the risk estimates, reflect uncertainty in the risk analysis construct and primarily regard the fits of the applied models to the data. The risk analysis construct for this analysis involved the use of PRZM/EXAMS model exposure data and laboratory toxicity data as fit by a log-probit model. As noted above these uncertainty estimates reflect only a portion of the true uncertainty. However, the uncertainty evaluated herein does address the fact that there is uncertainty in the estimates of risk indicated by the RQs, and is an effort to provide quantitative estimates of detrimental effect and reasonable bounds on those effect estimates.

VIII. Risk Characterization

Based on Risk Quotients (RQs), the deterministic risk assessment indicated that ChemX can pose a "high risk" to aquatic organisms. Based on the probabilistic analysis, the use of ChemX can be expected to infrequently (5% if the time or less) result in significant freshwater fish mortalities and may routinely result in reduced growth and other chronic effects in exposed fish. Substantial mortalities and chronic effects to sensitive aquatic invertebrates may be expected to commonly occur after peak exposures. Estuarine organisms, both fish and invertebrates, appear to be more sensitive than their freshwater relatives. Exposures in their habitat, such as tidal pools, bayous, salt marshes, tidal creeks, etc., which approximate exposures predicted in farm ponds would be expected to result in high mortality to these animals. Such related exposures are reasonable and plausible.

There are many uncertainties associated with the refined assessment, which were not directly addressed within the assessment including uncertainty associated with extrapolating from laboratory to field effects, and the use of exposure model derived estimated environmental concentrations (EECs) to represent actual concentrations. The uncertainties that were addressed in the probabilistic analyses, and which are included in the bounds given for the risk estimates, reflect uncertainty in the risk analysis construct and primarily regard the fits of the applied models to the data. However, the uncertainty evaluated does address the fact that there is uncertainty in the estimates of risk indicated by the RQs, and is an effort to provide quantitative estimates of detrimental effect and reasonable bounds on those effect estimates.

Literature studies indicate that sublethal effects on fish from acute exposures to ChemX can be expected due to the class and the mode of action of the chemical. These endpoints are generally not assessed by the standard toxicity test protocols used by EFED, and so are not included in this probabilistic case study. If dose-response data were available for sublethal ChemX effects were availabel, these endpoints could be included in a probabilistic assessment using the model employed here.

The high probability of mortality to sensitive invertebrates like zooplankton and macroarthropods will likely have an indirect effect on fish and other higher trophic level organisms. Additionally, the high probability of exceeding aquatic invertebrate chronic "no effect" concentrations would also contribute to these indirect effects. Such indirect effects on fish and other tertiary or higher consumers could include reduced juvenile survival due to reduced food resources, alterations in fish population structure, decreases in fish numbers, stunting or other size related effects in the population, etc.

ChemX is well known for the hazard it poses to birds and has a lengthy incident report history to warrant grave concern for those animals. The incident history for fishes is relatively scant in comparison, and the probabilistic analysis explains that large die-offs would be an infrequent, though real, occurrence. Invertebrates can be expected to suffer more routine mortalities and other ill effects, although these would be unlikely to be captured in an incident report due to their subtlety. Similarly, sublethal and chronic effects to fishes would not be tractable through incident reports. Nevertheless, flowable uses of ChemX do pose real and significant risks, acutely and chronically, to aquatic organisms.

IX. References

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Appendix A: 2-D Monte Carlo Model for the Analysis of Aquatic Risks

Introduction

The following discussion outlines the statistical basis for the joint probability function between exposures and risk. Consider the function of the single random variable $Y = g(X)$. The function $g(x)$ is assumed to be a monotonically increasing function of x with unique inverse $g^{-1}(y)$. When $Y = y$, $x = g^{-1}(y)$. The cumulative distribution function (CDF) for Y is given by

$$F_Y(y) = F_X[g^{-1}(y)]$$

For continuous X, and $X \geq 0$, the CDF for Y is then

$$F_Y(y) = \int_{x \leq g^{-1}(y)} f_X(x)\,dx = \int_0^{g^{-1}(y)} f_X(x)\,dx$$

Now consider the log-probit dose-response model,

$$r = \Phi(Z) \qquad where \qquad Z = intercept + slope \cdot \log_{10}(C)$$

where r is the measure of risk, C is the measure of dose appropriate for the dose-response function (e.g., exposure, concentration, etc.), and $\Phi(x)$ is the standard normal cumulative distribution function. When the dose is a random variable, that is, dose exhibits stochastic variation due to natural fate and transport processes, then risk itself is also a random variable characterized by its own cumulative distribution function (CDF) which is dependent on the distribution of exposures. When C is a random variable, the distribution of risks can be expressed using the first two equations above. The inverse function for the log-probit is then

$$C = g^{-1}(r) \doteq \gamma(r) \qquad where \qquad \gamma(r) = \exp\left[\ln(10)\,\frac{\Phi^{-1}(r) - intercept}{slope}\right]$$

and the distribution of risks is

$$F_R(r) = \int_0^{\gamma(r)} f_C(c)\,dc = F_C[\gamma(r)]$$

where $f_C(c)$ is the probability density function for exposure (dose, concentration). If exposures are lognormally distributed, $C \sim LN(\mu,\sigma)$, the distribution of risks for a log-probit dose-response model can be expressed in terms of the standard normal distribution function

$$F_R(r) = \Phi\left(\frac{\ln[\gamma(r)] - \mu}{\sigma}\right) = \Phi\left[\frac{1}{\sigma}\left(\ln 10\,\frac{\Phi^{-1}(r) - intercept}{slope} - \mu\right)\right]$$

For distributional forms of exposures other than lognormal, $F_C(c)$, the distribution of risks is

$$F_R(r) = F_C[\gamma(r)]$$

where $F_C(c)$ is the relevant distribution of doses.

Case I. Modeling the Distribution of Peak Concentrations Using Theoretical Distributions Functions.

Variability in Peak Exposures

Peak concentration data from each PRZM-EXAMS run were fit using commercial fitting software *ExpertFit*™ (Averill M. Law & Associates). *ExpertFit*™ provides a extensive selection of non-negative, continuous distributions which can take on a wide variety of shapes: chi-square, Erlang, exponential, F, gamma, inverse Gaussian, inverted Weibull, log-Laplace, log-logistic, pareto, lognormal, Pearson Type 5, Pearson Type 6, random walk, Rayleigh, Wald, and Weibull. Generally, non-negative continuous distributions are of the form

$$C \sim F(\gamma, \alpha, \beta)$$

where ~ is read as "*is distributed as*", γ is a location parameter, α is a shape parameter, and β is a scale parameter. For this analysis, location parameters were taken as zero, $\gamma = 0$, so that peak concentration data were fit as $C \sim F(\alpha,\beta)$. *ExpertFit*™ uses maximum likelihood estimation methods and provides an heuristic score and ranking of the overall quality of fit. The asymptotic variance-covariance matrix for the estimated parameters of the distribution is also provided. It provides the basis for quantitatively characterizing the uncertainty in fit.

Uncertainty in Peak Exposures

Uncertainty in the variability of peak concentrations was assumed to captured in the uncertainty in its shape and scale parameters (α,β) of the best fitting distribution. Parameter uncertainty was modeled as bivariate normal, that is,

$$(\alpha, \beta) \sim BiN(\mu_\alpha, \sigma_\alpha, \mu_\beta, \sigma_\beta, \rho)$$

where $(\mu_\alpha, \sigma_\alpha, \mu_\beta, \sigma_\beta, \rho)$ are the means, standard errors, and correlation coefficient for the bivariate normal uncertainty distribution derived from the asymptotic variance-covariance matrix of the maximum likelihood estimates.

Case II. Modeling the Distribution of Peak Exposures Using a Mixed Empirical-Exponential Distribution.

Given the complicated stochastic nature of historical rainfall pattens which drive PRZM-EXAMS output, it is not surprising that a single family of theoretical distributions could not be fit to the PRZM-EXAMS data and that the quality of fit varied widely among scenarios. In order to test the dependency of the exposure-risk joint probability function, a 2-D Monte Carlo simulation model was developed which was based on the empirical distribution function (EDF) rather than a fitted theoretical distribution.

One shortcoming using the PRZM-EXAMS output as an EDF is that it most likely does not represent the right tail of the true underlying distribution very well. The algorithm presented below uses a piece-wise linear empirical distribution function for the first $n-k$ observations and a shifted exponential to the right of the C_{n-k}^{th} peak exposure. The exponential parameter is chosen so that the means from the overall fitted distribution and the mean from the PRZM-EXAMS output are the same. There is some theoretical support for representing the right tail of a long-tailed distribution with an exponential distribution (see Bratley *et. al*. , page 133, Theorem 4.71). For this analysis, the right, exponential tail was truncated at 10 times the maximum peak, based on best professional judgement. The EDF minimum was set at zero, with a linear extrapolation from the model-estimated minimum.

The following section outlines the algorithm used to generate random variates from a mixed empirical-exponential distribution.

<u>Mixed Empirical-Exponential Distribution</u> (see Bratley *et. al*. pages 131-135, and 150-151). The peak concentrations (annnual maxima) from a given PRZM-EXAMS run are sorted so that $C_1 \le C_2 \le \cdots \le C_n$. A piece-wise linear CDF is then fit to the first $n-k$ observations and a shifted exponential CDF is fit to the largest k observations. Taking $F(0) = 0$ and defining $C_0 = 0$, the CDF is then

$$F(t) = \frac{i}{n} + (t - C_i)\,[n\,(C_{i+1} - C_i)] \quad \textit{for} \quad C_i \le t \le C_{i+1}$$

$$F(t) = 1 - \frac{k}{n}\exp\left[-\frac{1}{\theta}(t - C_{n-k})\right] \quad \textit{for} \quad t > C_{n-k}$$

for $i = 0, 1, \cdots, n-k-1$ and where

$$\theta = \frac{1}{2k}C_{n-k} + \frac{1}{k}\sum_{i=n-k+1}^{n}(C_i - C_{n-k})$$

The algorithm for generating a mixed empirical-exponential variate is based on inversion of the CDF and is given by Bratley (pg. 151) as:

(1). Generate a uniform random variate on (0,1)

$U \quad U(0,1)$

(2). if $U > 1 - k/n$, then return

$C = C_{n-k} - \theta \log\,[n\,(1-U)/k\,]$

(3) otherwise set $V \quad nU$, $I \quad \lfloor V \rfloor$ and return

$C = (V-I)\,(C_{I+1} - C_i) + C_I$

where $\lfloor Y \rfloor$ is the floor function which returns the largest integer not great than Y.

Figure 12. Typical Exposure Distribution

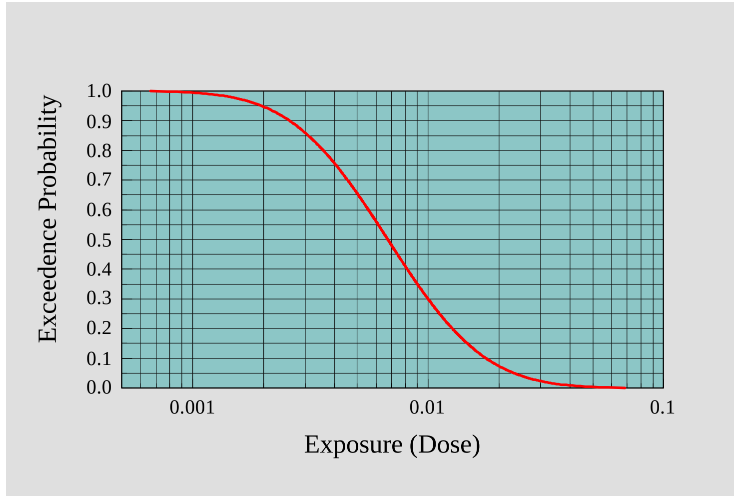


Figure 13. Log-probit dose response function

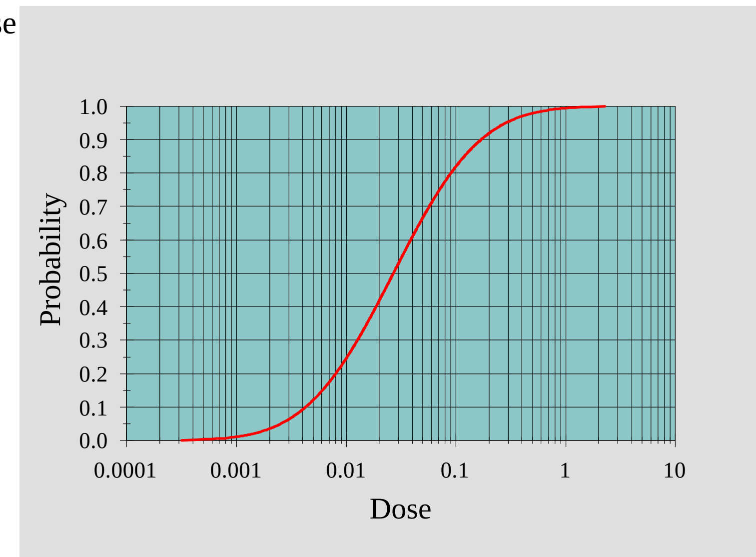
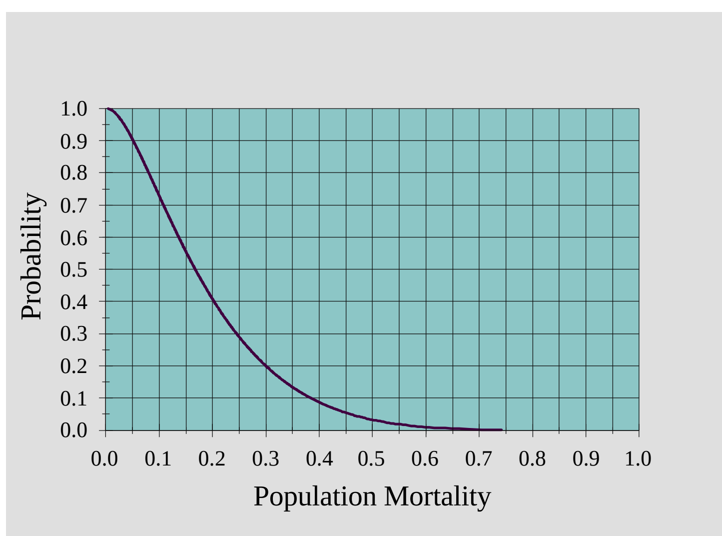


Figure 14. Joint Probability function combining dose distribution and dose-response function.



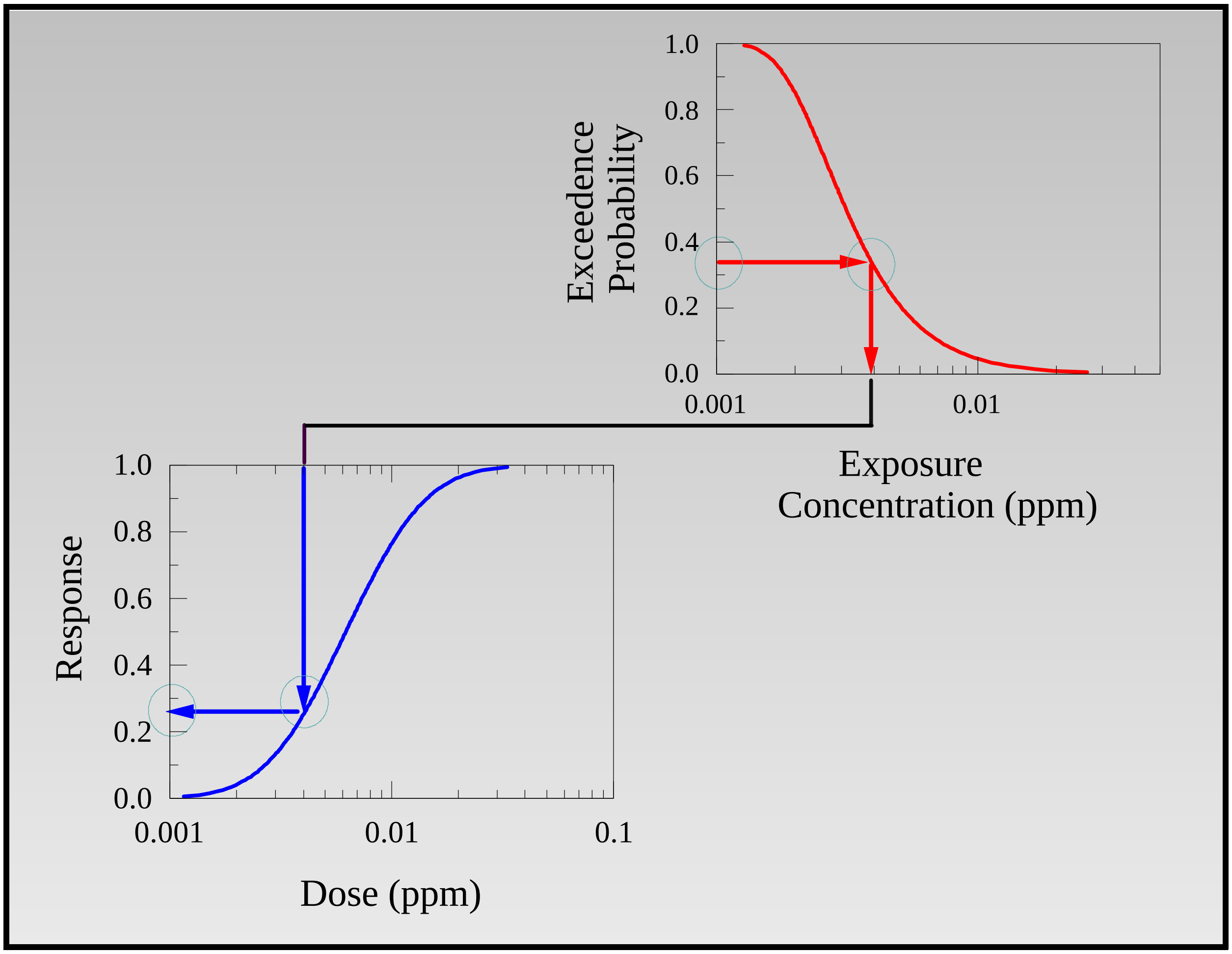
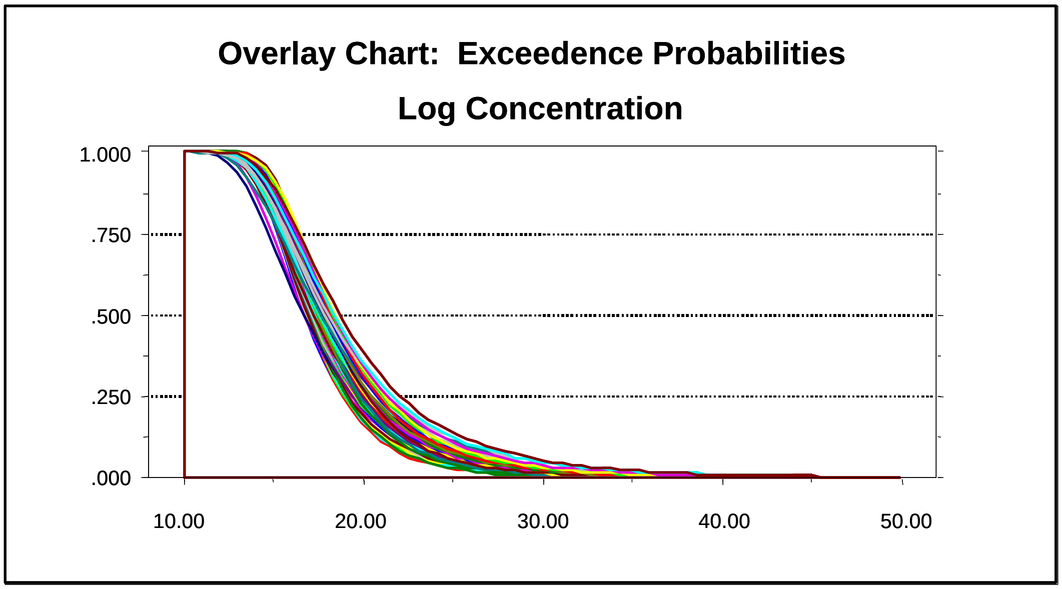
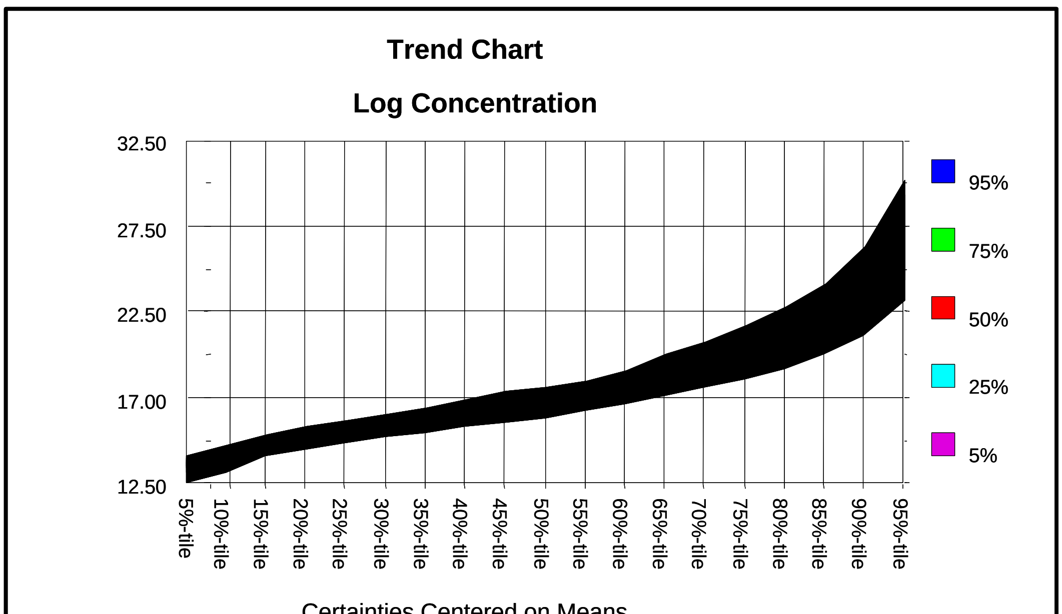


Figure 15: Graphical represenation of calculation of response

Figure 16(Top). Example of the uncertainty in the distribution of peak concentrations. Each of the 50 CCDFs (Complementary Cumulative Distribution Functions) represents a different realization of the exceedence distribution for a fitted gamma density. The uncertainty is modeled from the asymptotic variance-covariance matrix for the maximum likelihood parameters of the of the fitted gamma distribution.

Figure 17(Bottom). The trend chart shows confidence bounds based on percentiles of the fitted gamma distribution.





Appendix B: EPA C Program Code

```
/* -----------------------------------------------------------------
   Program to generate the joint probability function for aquatic risks
   The Dose-response function is modeled as log-probit,
     risk = N(z)
     z = intercept + slope * log10(exposure)
   Exposure data is from Prizm-Exams.  The exposure distribution is a
   mixed empirical-exponential CDF with the number of points in the
   upper tail is specified by the user.

   Program is set up to run in Batch or non-Batch mode

   Date:  09.13.2000

   by:    Timothy Barry
    barry.timothy@epa.gov
    202-260-2038
   -----------------------------------------------------------------
*/

#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <time.h>
#include "nr.h"                  /*Numerical Recipes header files*/
#include "nrutil.h"              /*Numerical Recipes utility header files*/
#include "nrutil.c"              /*Numerical Recipes utilities*/

#include "dsort.c"               /*sort array routine*/
#include "dsort2.c"              /*sort first array, carry second*/
#include "dmsort.c"              /*matrix sort*/
#include "mean_var.c"            /*mean and variance of an array*/
#include "get_seed.c"            /*random seed*/
#include "ranlib.c"              /*short library of random number routines*/
#include "edf_dist.c"            /*mixed EDF-Exponential tail functions*/
#include "avnlib.c"              /*statistical functions*/
#include "bootstrp.c"            /*bootstrap an array*/
#include "lround.c"              /*rounding long integers*/

#define N  36                    /*number of yearly peak concentrations*/
#define K0 3                     /*number of points in the exponential tail*/
#define NP  1000                 /*points in 1-D Monte Carlo*/
#define NPR 999                  /*number of probabilities written*/
                   /*to 2-D output file*/

FILE *fptr0,*fptr1,*fptr2,*fptr3;      /*input, output files*/
long rseed,inner,outer;
time_t start_time,end_time,seed_time;  /*program execution timing parms*/
static double VPROB[5] =               /*uncertainty fractiles*/
   {0.05,0.25,0.50,0.75,0.95};

void Report(double **s, double p[], double min, double max);

int main(int argc, char *argv[])
{
   int batch;
   long i,j,k,*year,seed,indx;
   char title[50];
   char outfile[3][12];
```

```
double **stats;
double y0,*peak,c1,c2,c3,c4,c5,c6;
double slope,se_slope,intercept,se_intercept,rho;
double pr,theta,mean,*ave,var,*dose,*risk,z,*boot;
double ran_slope,ran_intercept,mindose,maxdose;

peak = dvector(1,N);                /*array of peak concentrations*/
year = lvector(1,N);                /*year*/
boot = dvector(1,N);                /*array for bootstrap sample*/

if (argc!= 3) nrerror("Command Line Failure");
if ((fptr0 = fopen(argv[1],"r"))==NULL)
   nrerror("Opps: Could not Open input file");
batch = atoi(argv[2]);
if (!batch)
   printf("\n Non-batch Mode\n");
else
   printf("\n Program in Batch Mode\n");

fscanf(fptr0,"%s\n",&title);
fscanf(fptr0,"%s\n",outfile[0]);
fscanf(fptr0,"%s\n",outfile[1]);
fscanf(fptr0,"%s\n",outfile[2]);
fscanf(fptr0,"%ld %ld\n",&outer,&inner);

if ((fptr1= fopen(outfile[0],"w"))==NULL)
   nrerror("Opps.  Could not open Output file");
if ((fptr2= fopen(outfile[1],"w"))==NULL)
   nrerror("Opps.  Could not open Output file");
if ((fptr3= fopen(outfile[2],"w"))==NULL)
   nrerror("Opps.  Could not open Output file");

printf("\n %s",title);
printf("\n ---------------------------------------------");
printf("\n User-specified Output Files:");
printf("\n      %s",outfile[0]);
printf("\n      %s",outfile[1]);
printf("\n      %s",outfile[2]);
printf("\n User-specified Simulations");
printf("\n ---------------------------------------------");
printf("\n     %5ld outer realizations",outer);
printf("\n     %5ld inner simulations\n",inner);

printf("\n Dose-Response Parameters");
printf("\n ---------------------------------------------");
fscanf(fptr0,"%lf %lf\n",&intercept,&se_intercept);
fscanf(fptr0,"%lf %lf\n",&slope,&se_slope);
fscanf(fptr0,"%lf\n",&rho);
fscanf(fptr0,"%lf %lf",&mindose,&maxdose);

printf("\n   Slope,SE(slope)           %9.5lf %9.5lf",slope,se_slope);
printf("\n   Intercept, SE(intercept)  %9.5lf %9.5lf",intercept,se_intercept);
printf("\n   Rho                       %9.5lf\n",rho);
if(!batch) message_p("\nReturn to Continue:");

for (k=1;k<=N;k++)
   fscanf(fptr0,"%lf\n",&peak[k]);
dsort(N,peak);                        /*make sure peak data are sorted*/
mean_var(peak,N,&mean,&var);           /*get mean and variance for peak data*/
printf("\n Yearly Peak Concentrations");
printf("\n ---------------------------------------------");
```

```
for (k=1;k<=12;k++)
   printf("\n %4ld %8.3lf     %4ld %8.3lf     %4ld %8.3lf",3*k-2,
      peak[3*k-2],3*k-1,peak[3*k-1],3*k,peak[3*k]);
printf("\n\n Sample mean, var:            %9.3lf %9.3lf",mean,var);
printf("\n Minimum allowed concentration %9.3lf",mindose);
printf("\n Maximum allowed concentration %9.3lf\n\n",maxdose);

if(!batch) message_p("\nReturn to continue ...");

/*Begin 1D Simulation with basic input data*/
/*----------------------------------------*/
   theta = Mixed_EDF_Tail_Mean(N,K0,peak);
   seed = Get_Seed();
   dose = dvector(1,NP);
   risk = dvector(1,NP);
   for (k=1;k<=NP;k++)
   {
      y0 = 0.0;
      do {
            pr   = dran1(&seed);
            y0 = Mixed_EDF_Inverse(N,K0,peak,theta,pr);
         } while ((y0 < mindose) || (y0 > maxdose));
         dose[k]=y0;
         z = intercept + slope*(log10(dose[k]));
         risk[k] = pnorm(z);
   }
   dsort2(NP,dose,risk);
   fprintf(fptr1,"dose, risk, probability\n");
   for (k=1;k<=NP;k++)
      fprintf(fptr1,"%12.6le %12.6le %9.6lf\n",dose[k],risk[k],k/(NP+1.0));

/*Begin 2D Simulations                    */
/*------------------------------------------*/
   indx=1;
   free_dvector(dose,1,NP);
   free_dvector(risk,1,NP);
   dose = dvector(1,inner);
   risk = dvector(1,inner);
   stats = dmatrix(1,6,1,outer);            /*save 6 uncertain statistics*/
   ave = dvector(1,outer);
   start_time = time(NULL);                 /*get program starting time*/
   rseed=seed;
   for (j=1;j<=outer;j++)                  /*begin outer loop*/
   {
      Boot_Simple(N,peak,boot,indx,&seed);    /*boot = simple bootstrap sample*/
      theta = Mixed_EDF_Tail_Mean(N,K0,boot); /*calc theta ...see Bratley et. al.*/

      /*get bivariate normal random variates*/
      BiNorm(slope,se_slope,intercept,se_intercept,rho,&ran_slope,&ran_intercept,&seed);
      if (!(j%250))
         printf("%5ld %9.4lf\n",j,(double)j/outer);
      for(k=1;k<=inner;k++)                /*Begin inner loop*/
      {
         y0 = 0.0;
         do {                          /*loop until min <= dose <= max*/
               pr = dran1(&seed);
               y0 = Mixed_EDF_Inverse(N,K0,boot,theta,pr);
            } while ((y0 < mindose) || (y0 > maxdose));
         dose[k]=y0;
         z = ran_intercept + ran_slope*(log10(dose[k]));
         risk[k] = pnorm(z);
```

```
        }
        mean_var(risk,inner,&mean,&var);
        ave[j]=mean;
        dsort(inner,risk);

        /*save jth realization of key statistics*/
        /*--------------------------------------*/
          for (k=1;k<=5;k++)
            stats[k][j] = risk[lround(VPROB[k-1]*inner)];
          stats[6][j] = mean;
      }
      printf("\n Sorting ...");
      dMsort(stats,6,outer);
      dsort(outer,ave);
      for (k=1;k<=NPR;k++)
      {
        pr = k/(NPR+1.0);           /*use Weibull plotting position*/
        indx=lround(pr*outer);
        fprintf(fptr2,"%10.5lf %10.5lf",pr,1-pr);
         for (i=1;i<=6;i++)
          fprintf(fptr2,"  %10.4le",stats[i][indx]);
         fprintf(fptr2,"\n");
      }
      end_time = time( NULL );
      message("Printing Report");
      Report(stats,peak,mindose,maxdose);
      printf("\n Successful Completion\n\n");

      free_dvector(dose,1,inner);
      free_dvector(risk,1,inner);
      free_dmatrix(stats,1,6,1,outer);
      fclose(fptr0);
      fclose(fptr1);
      fclose(fptr2);
      return 0;
}

void Report(double **s, double p[], double min, double max)
{
   long i,j,k,indx;
   double pr,w,mean,var;
   end_time = time( NULL );
   mean_var(p,N,&mean,&var);
   fprintf(fptr3,"\Summary Statistics\n");
   fprintf(fptr3,"-------------------------------------------------------\n");
   fprintf(fptr3," Starting Time:              %s",ctime(&start_time));
   fprintf(fptr3," Finishing Time:             %s",ctime(&end_time));
   fprintf(fptr3," Computation Time (minutes):  %10.2f\n",(difftime(end_time,start_time))/60.0);
   fprintf(fptr3," Random Number Seed:         %10ld\n",rseed);
   fprintf(fptr3," Realizations:               %10ld\n",outer);
   fprintf(fptr3," Simulations:                %10ld\n",inner);
   fprintf(fptr3," Total Number of Monte Carlo Simulations:  %ld\n",inner*outer);

   fprintf(fptr3,"\n\n Sorted Peak Concentrations");
   fprintf(fptr3,"\n -----------------------------------------------");
   for (k=1;k<=12;k++)
      fprintf(fptr3,"\n %4ld %8.3lf     %4ld %8.3lf     %4ld
%8.3lf",3*k-2,p[3*k-2],3*k-1,p[3*k-1],3*k,p[3*k]);
   fprintf(fptr3,"\n\n Sample mean, var:    %9.3lf %9.3lf",mean,var);
   fprintf(fptr3,"\n Minimum allowed con. %9.3lf",min);
   fprintf(fptr3,"\n Maximum allowed con. %9.3lf\n",max);
```

```
   fprintf(fptr3,"\n                                    PDFv");
   fprintf(fptr3,"\n  PDFu");
   for (k=0;k<=4;k++)
      fprintf(fptr3,"   %9.3lf",VPROB[k]);
   fprintf(fptr3,"      Mean");
   fprintf(fptr3,"\n
-----------------------------------------------------------------------------\n");
   for (i=1;i<=39;i++)
   {
      pr = i/40.0;
      fprintf(fptr3,"%7.3lf ",pr);
      indx = i*outer/40;
      for (k=1;k<=6;k++)
         fprintf(fptr3,"   %8.2le",s[k][indx]);
      fprintf(fptr3,"\n");
   }
   fprintf(fptr3,"\n  Mean  ");
   for (k=1;k<=6;k++)
   {
      mean_var(s[k],outer,&mean,&var);
      fprintf(fptr3,"   %8.2le",mean);
   }
}


#undef N
#undef K0
#undef NP
#undef NPR
```

Appendix C: Crystal Ball Program - Data Entry Template

Distribution of Individual Risks

Model Parameter		Distributional Parameters	Best	SE
Concentration	shape	6.473672	6.37051	0.8278
Parameters	scale	2.3532403	16.40963	0.4520
		correlation	-0.3131	
Dose-Response	Intercept	-7.22343	-10.601	0.148
log-normal	Slope	2.59235	5.550	1.175
		correlation	-0.993	

Uniform	0.092527	
Ohio Corn	20.582047	inversion
Z	-3.818398	
5th% Fish	0.000067	

Key change here for each new fit

Appendix D: EPA C-Based Monte Carlo Program - Data Entry Template, Annotated

ChemX_Bluegill_MSCotton_MaxRate	**> Title**
bMSCtBG.txt	**> Output File 1**
cMSCtBG.txt	**> Output File 2**
rMSCtBG.txt	**> Output File 3**
2500 5000	**> Number of Inner and Outer Loop Simulations**
-13.618525 2.414178	**> Intercept of Probit Dose-Response Curve**
6.75501353 1.218704	**> Slope of Probit Dose-Response Curve**
-0.997	**> Correlation of Dose-Reposnse Parameters**
0.0 94.06	**> Exposure Minimum and Maximum**
0.34	**> Exposure Model Data From PRZM/EXAMS**
0.375	
0.379	
0.858	
1.179	
1.218	
1.709	
2.161	
2.201	
2.558	
2.58	
3.006	
3.096	
3.136	
3.465	
4.41	
4.874	
4.935	
5.523	
5.715	
6.067	
6.168	
7.156	
...	
37.11	
47.03	

Appendix E: Best-Fit Distributions to Exposure Model Peak Data

Best Fit for Yearly Peak Data

Data Set	Best Fit Distribution	Parameters	MLE	Var	Covar	SIG	Rho
Maine Potato 1	Inverted Weibull	Scale	23.51384	0.32749	-0.16788	0.57227	-0.31308
		Shape	7.21065	0.87801		0.93702	
Maine Potato 2	Lognormal	Scale	1.77768	0.01726	0.00000	0.13138	
		Shape	0.78833	0.00888		0.09424	
Mississippi Cotton	Log-Logistic	Scale	4.64067	0.72593	0.00000	0.85202	
		Shape	1.57233	0.43222		0.65743	
Ohio Corn 1	Inverted Weibull	Scale	16.40963	0.20434	-0.11716	0.45204	-0.31308
		Shape	6.37051	0.68533		0.82785	
Ohio Corn 2	(1). Random Walk	Scale	0.23185	0.00104	0.00000	0.03225	
		Shape	0.33291	0.00616		0.07847	
	(2). Log-Logistic	Scale	5.69811	0.47719	0.00000	0.69079	
		Shape	2.38120	0.99131		0.99565	
California Grape	Gamma	Scale	60.83855	309.44796	-1.51682	17.59113	-0.68772
		Shape	0.63046	0.01572		0.12538	
Florida Potato 1	Log-Logistic	Scale	42.05215	10.16931	0.00000	3.18894	0.00000
		Shape	3.80673	2.53350		1.59170	

Appendix E (continued) : Best-Fit Distributions to Exposure Model Peak Data

Iowa Corn Scenarios: Best Fits for Standard and Bounding Estimate Scenarios

Dataset	Scenario	Best Fit CDF	Parameters	MLE	Asymptotic Variance	Quality of Fit
3	pH 6.2, 90% Soil Aerobic Metabolism	lognormal	mu	4.43879	0.01072	OK
	Large Field:Pond Ratio		sig	0.62128	5.51E-03	
			covar		0	
7	pH 7, 90% Soil Aerobic Metabolism	Inverted Weibull	scale	21.59093	2.56652	OK
	Small Field:Pond Ratio		shape	2.36509	0.09446	
			Covar		-0.15415	
8	pH 7, 90% Soil Aerobic Metabolism	Inverted Weibull	scale	2.00823	0.07322	OK
	Medium Field:Pond Ratio		shape	23.28496	3.8509	
			Covar		-0.16624	
9	pH 7, 90% Soil Aerobic Metabolism	Inverted Gaussian	scale	63.36139	90.37039	OK
	Large Field:Pond Ratio		shape	78.18896	339.6396	
			Covar		0	
10	pH 7, 90% Soil Aerobic Metabolism	Inverted Weibull	scale	16.16171	0.13738	Cautious
	Standard Field:Pond Ratio		shape	7.65201	0.98878	
			Covar		-0.11539	
18	pH 9, Mean Soil Aerobic Metabolism	Pearson 5	scale	33.70807	68.14303	Cautious
	Small Field:Pond Ratio		shape	2.65081	0.34778	No fit available in CB
			Covar		4.42245	Not Modeled in CB

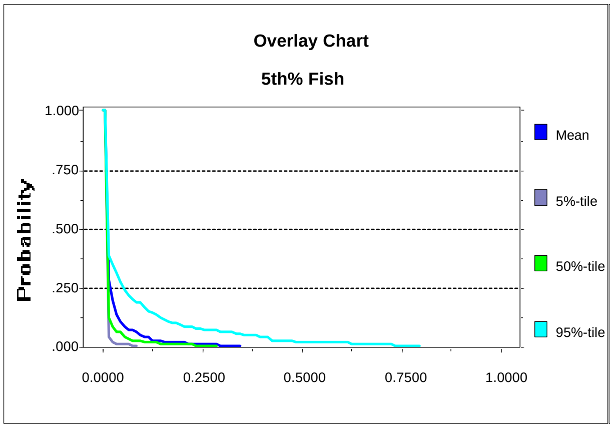
Appendix F: Toxicity Data Used in Monte Carlo Simulations

Species	Intercept (ppb)	Intercept Standard Error	Slope	Slope Standard Error	Correlation
Rainbow trout	-8.000	1.678	3.218	0.675	-0.988
Bluegill	-13.619	2.414	6.755	1.219	-0.997
5th Percentile Fish Species	–9.359	0.148	4.90	0.805	-0.993
50th Percentile Fish Species	-12.103	0.148	4.90	0.805	-0.993
Silvrerside	-3.057	0.475	2.053	0.342	-0.952
Daphnia magna	-8.812	1.111	5.790	1.228	-0.980
5th Percentile Invertebrate with Daphnia 25th Percentile	-5.478	2.940	5.790	1.228	-0.980
50th Percentile Invertebrate with Daphnia 25th Percentile	-10.644	2.940	5.790	1.228	-0.980
5th Percentile Invertebrate with Daphnia 50th Percentile	-3.207	1.270	5.790	1.228	-0.980
Pink shrimp	-4.975	1.111	5.970	1.228	-0/980

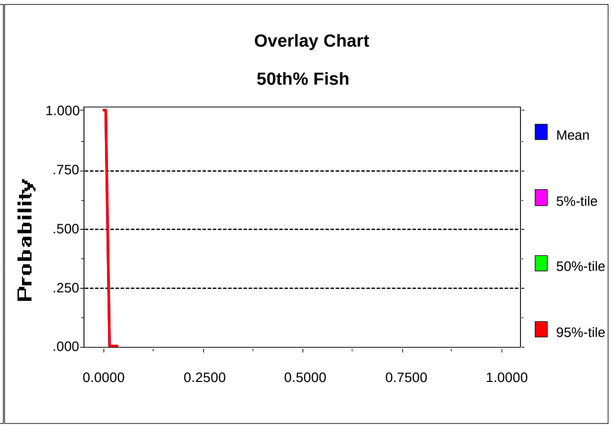
Appendix G: Graphs of Probability of Acute Mortality

Reverse Cumulative Distribution Function Graphs.
Individual risk is given on the x-axis of each graph. The percentiles indicate uncertainty bounds.

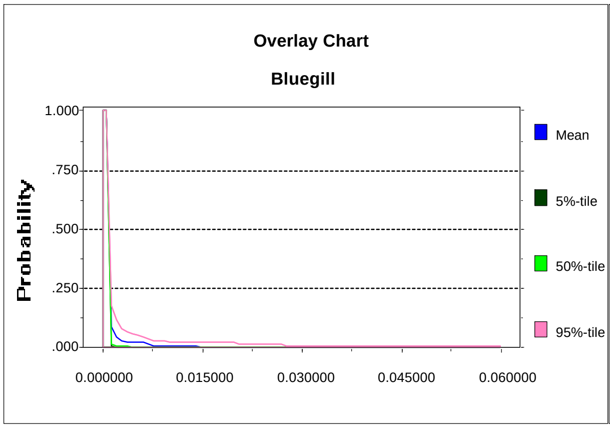
Ohio Corn: Fish



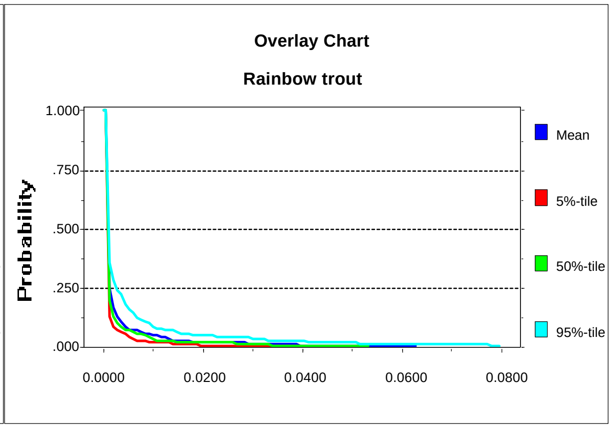
Ohio Corn: 5% Fish Species Mortality Following Peak Exposure to ChemX at the Maximum Rate



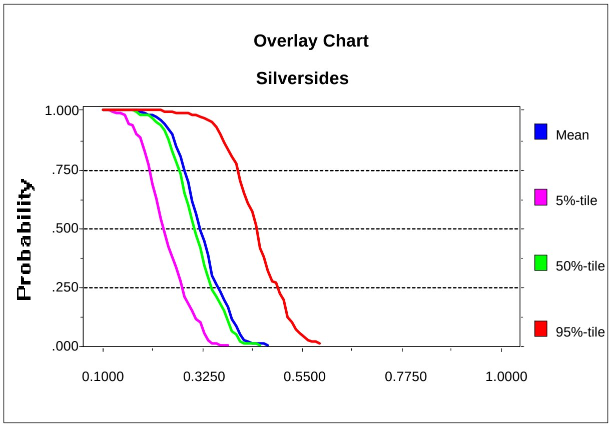
Ohio Corn: 50% Fish Species Mortality Following Peak Exposure to ChemX at the Maximum Rate



Ohio Corn: Bluegill Mortality Following Peak Exposure to ChemX at the Maximum Rate

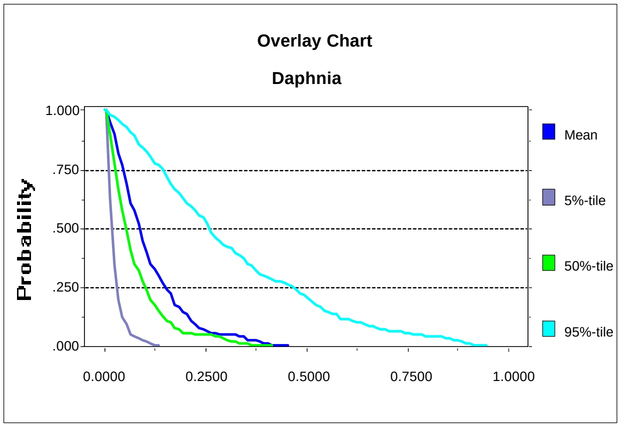


Ohio Corn: Rainbow Trout Mortality Following Peak Exposure to ChemX at the Maximum Rate

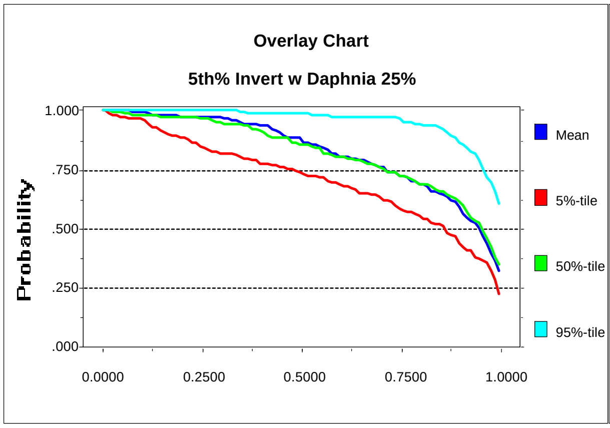


Ohio Corn: Silversides Mortality Following
Peak Exposure to ChemX at the Maximum Rate

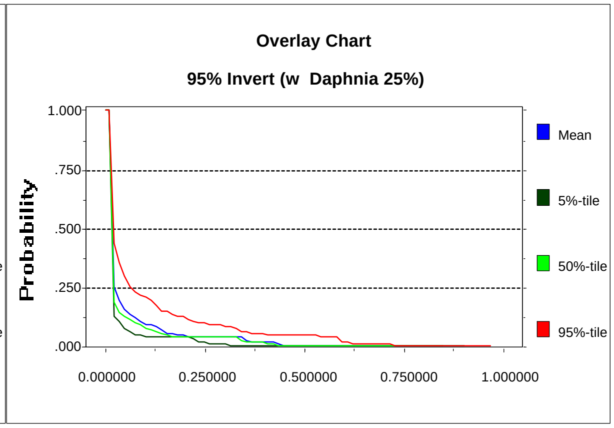
Ohio Corn: Invertebrates



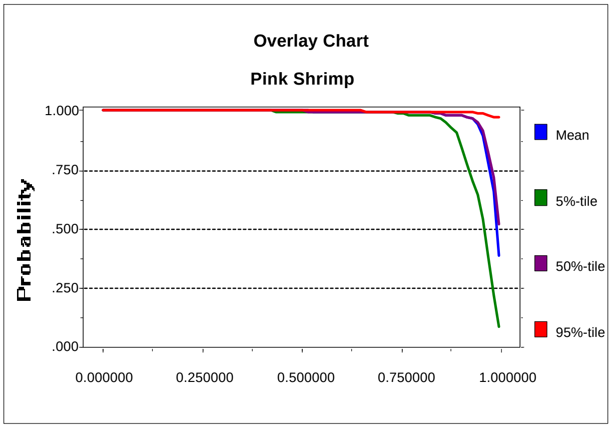
Ohio Corn: *Daphnia* Mortality Following
Peak Exposure to ChemX at the Maximum Rate



Ohio Corn: 5% Invertebrate Species
with *Daphnia* 25%, Mortality Following
Peak Exposure to ChemX at the Maximum Rate

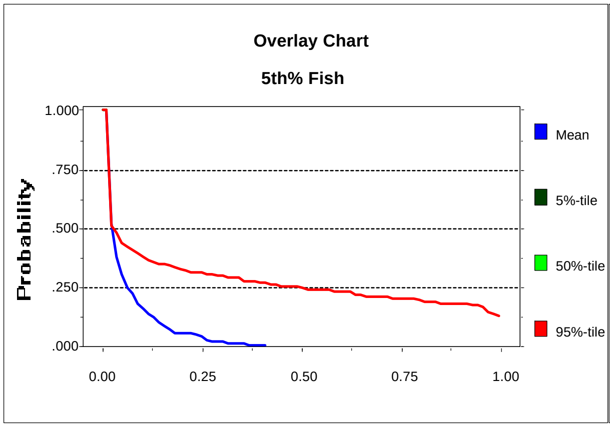


Ohio Corn: 50% Invertebrate Species
with *Daphnia* 25%, Mortality Following
Peak Exposure to ChemX at the Maximum Rate

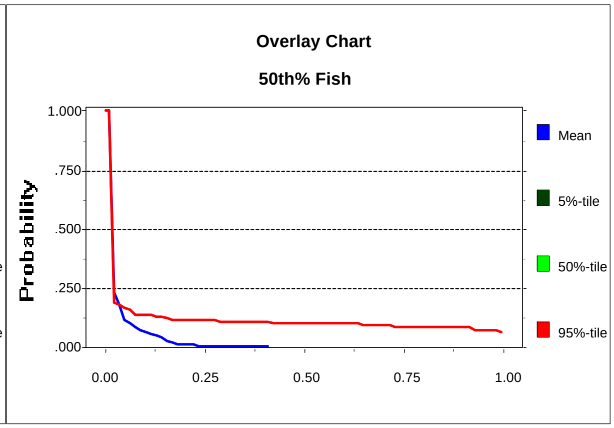


Ohio Corn: Shrimp Mortality Following
Peak Exposure to ChemX at the Maximum Rate

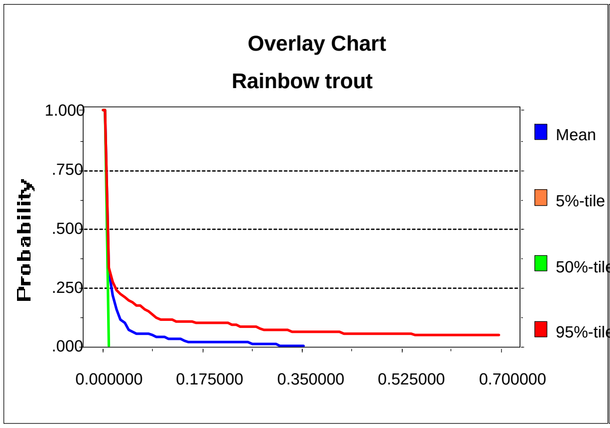
Mississippi Cotton: Fish



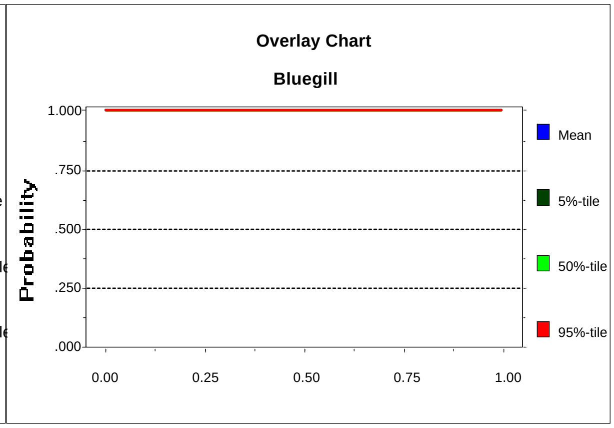
Mississippi Cotton: 5% Fish Species Mortality
Following Peak Exposure to ChemX
Used at the Maximum Rate



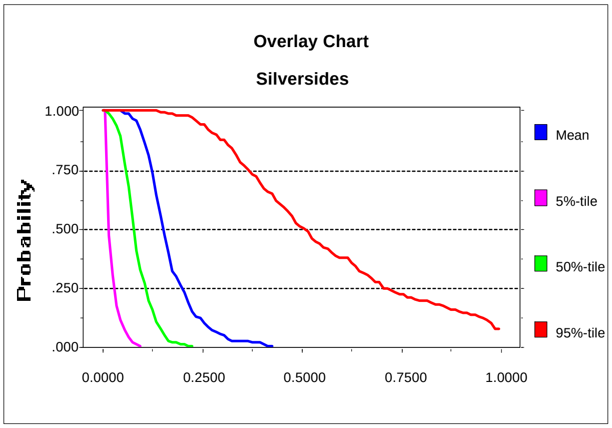
Mississippi Cotton: 50th% Fish Species Mortality
Following Peak Exposure to ChemX
Used at the Maximum Rate



Mississippi Cotton: Rainbow Trout Mortality
Following Peak Exposure to ChemX
Used at the Maximum Rate

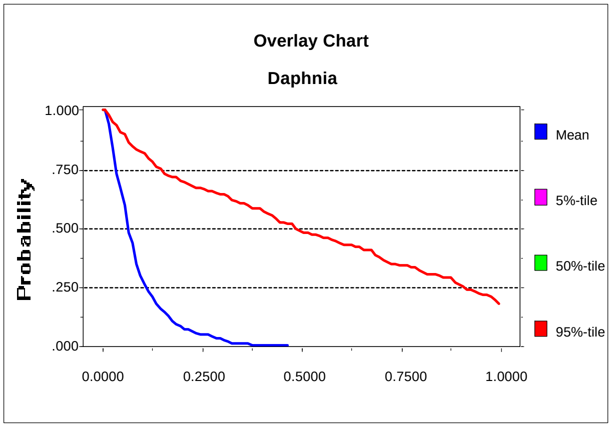


Mississippi Cotton: Bluegill Mortality
Following Peak Exposure to ChemX
Used at the Maximum Rate

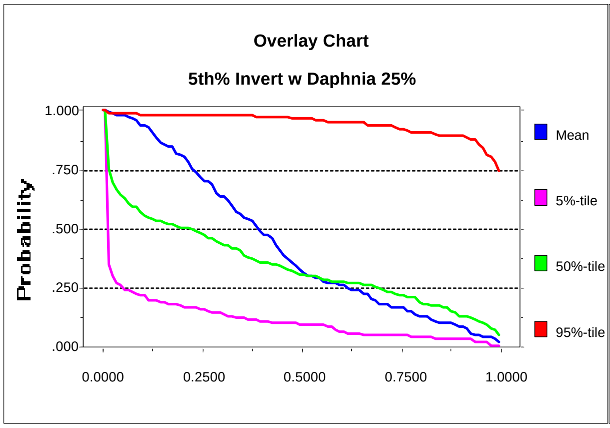


Mississippi Cotton: Silversides Mortality
Following Peak Exposure to ChemX
Used at the Maximum Rate

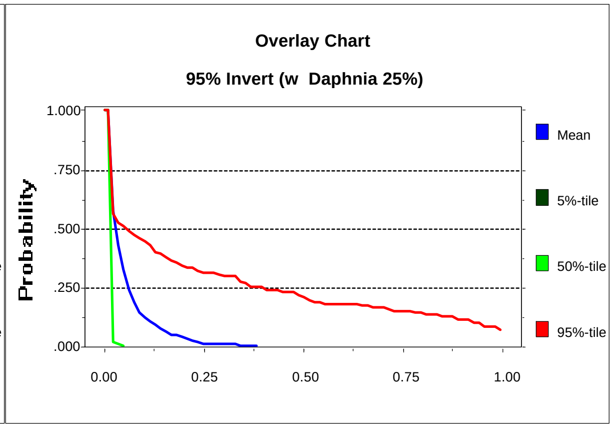
Mississippi Cotton: Invertebrates



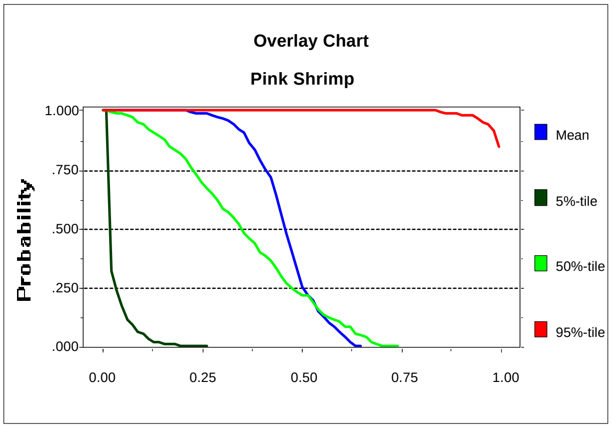
Mississippi Cotton: *Daphnia* Mortality Following Peak Exposure to ChemX at the Maximum Rate



Mississippi Cotton: 5% Invertebrates Species with *Daphnia* 25%, Mortality Following Peak Exposure to ChemX at the Maximum Rate

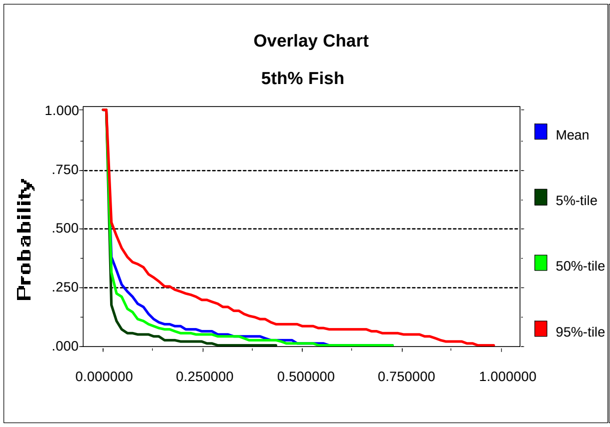


Mississippi Cotton: 50% Invertebrates Species with *Daphnia* 25%, Mortality Following Peak Exposure to ChemX at the Maximum Rate

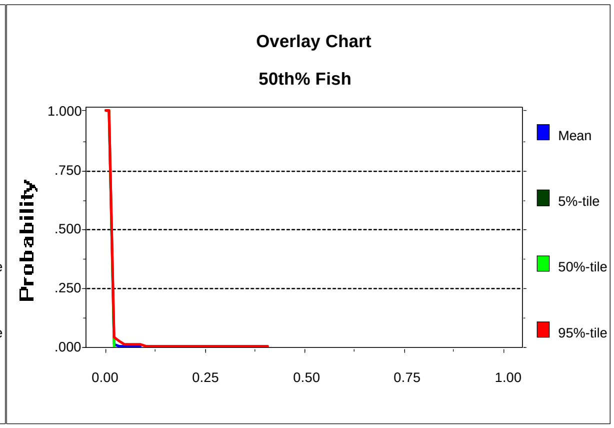


Mississippi Cotton: Shrimp Mortality Following Peak Exposure to ChemX at the Maximum Rate

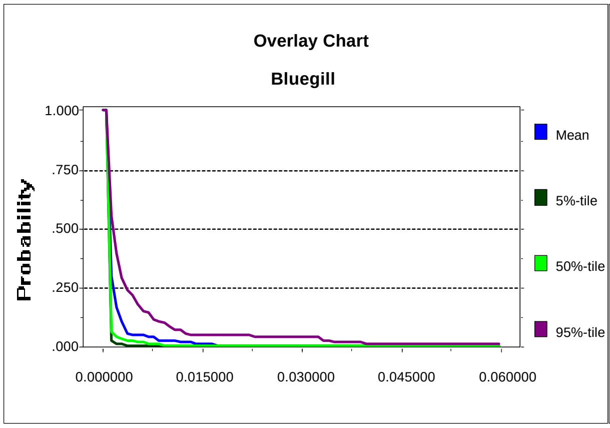
Maine Potatoes: Fish



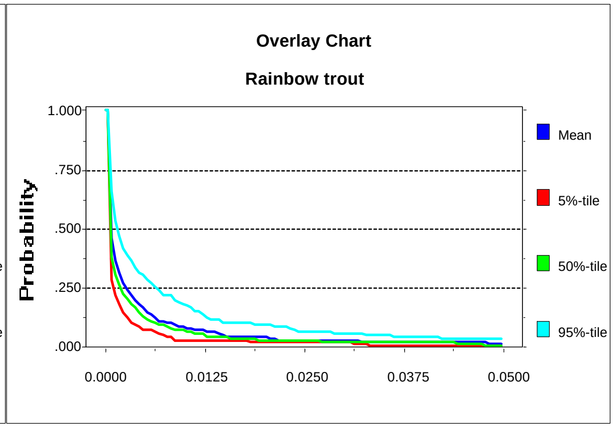
Maine Potatoes: 5% Fish Species Mortality Following Peak Exposure to ChemX Used at the Maximum Rate



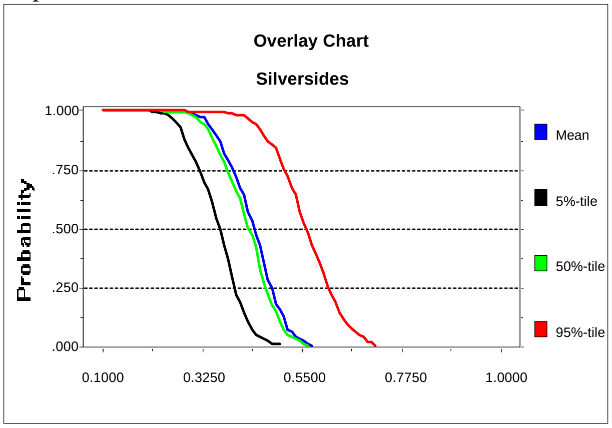
Maine Potatoes: 50th% Fish Species Mortality Following Peak Exposure to ChemX Used at the Maximum Rate



Maine Potatoes: Bluegill Mortality Following Peak Exposure to ChemX Used at the Maximum Rate

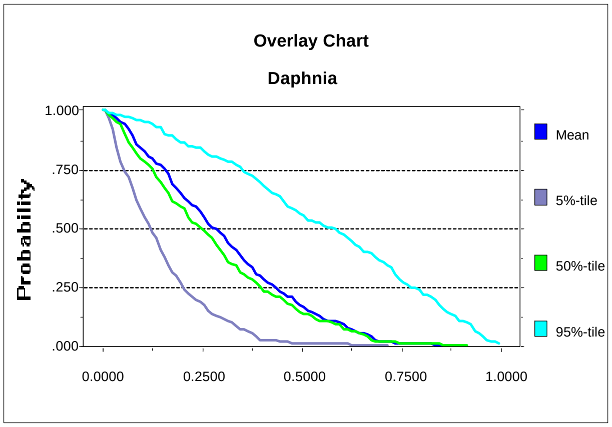


Maine Potatoes: Rainbow Trout Mortality Following Peak Exposure to ChemX Used at the Maximum Rate

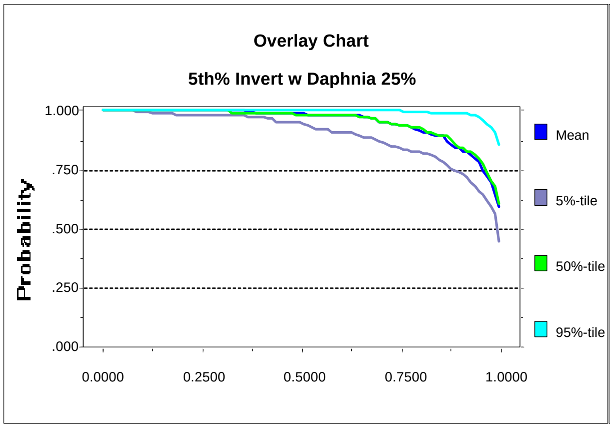


Maine Potatoes: Silversides Mortality Following Peak Exposure to ChemX at the Maximum Rate

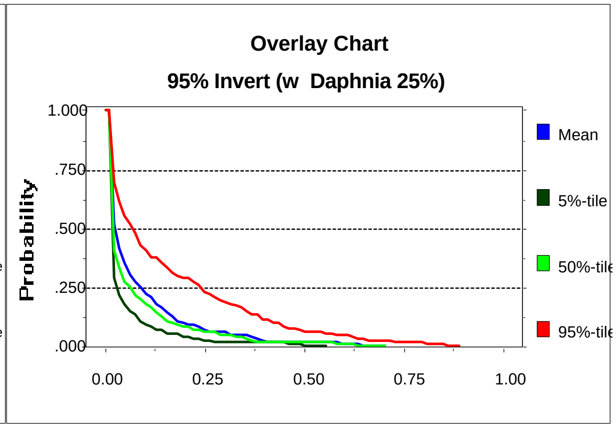
Maine Potatoes: Invertebrates



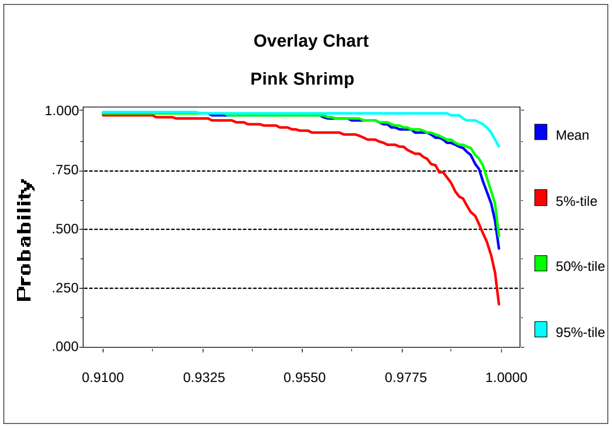
Maine Potatoes: *Daphnia* Mortality Following Peak Exposure to ChemX at the Maximum Rate



Maine Potatoes: 5% Invertebrate Species with *Daphnia* 25% Following Peak Exposure to ChemX at the Maximum Rate

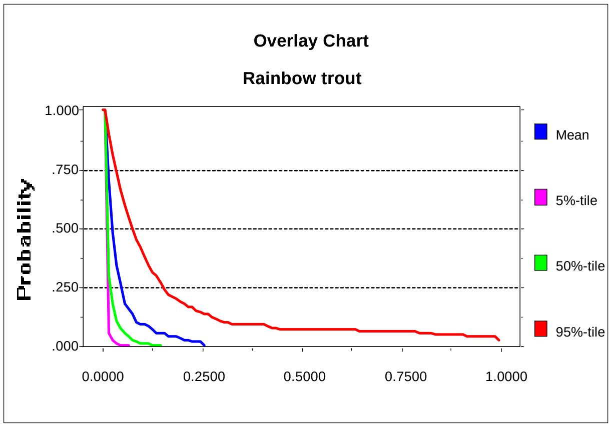


Maine Potatoes: 50% Invertebrate Species with *Daphnia* 25% Following Peak Exposure to ChemX at the Maximum Rate

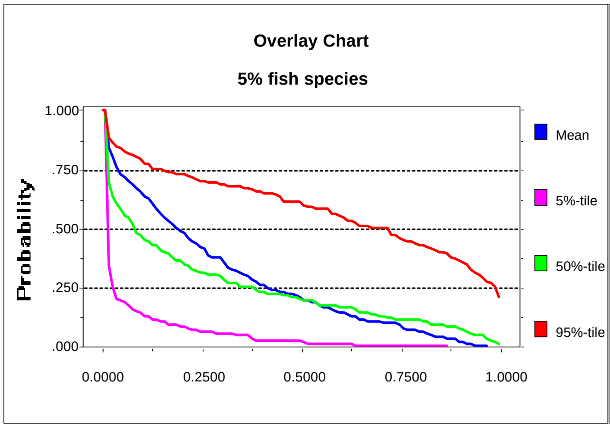


Maine Potatoes: Shrimp Mortality Following Peak Exposure to ChemX at the Maximum Rate

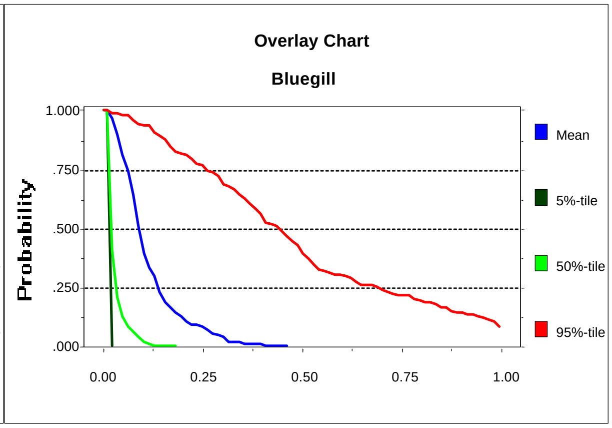
Florida Potatoes: Fish



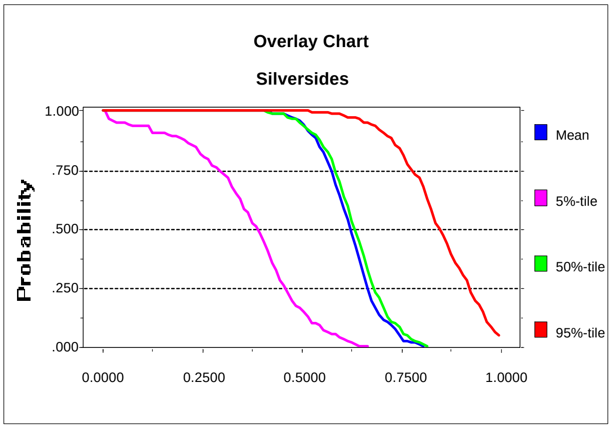
Florida Potatoes: Rainbow Trout Mortality Following Peak Exposure to ChemX at the Maximum Rate



Florida Potatoes: 5% Fish Species Mortality Following Peak Exposure to ChemX at the Maximum Rate

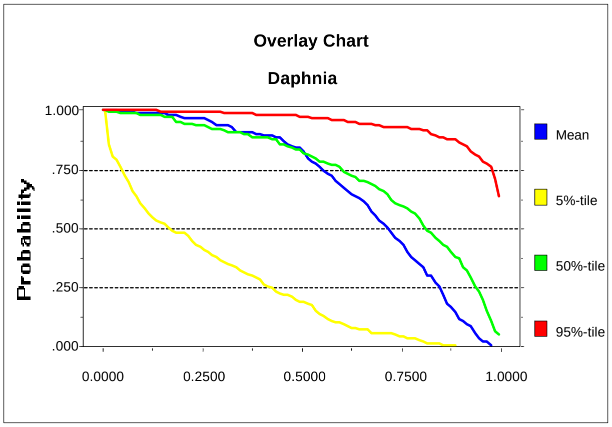


Florida Potatoes: Bluegill Mortality Following Peak Exposure to ChemX at the Maximum Rate

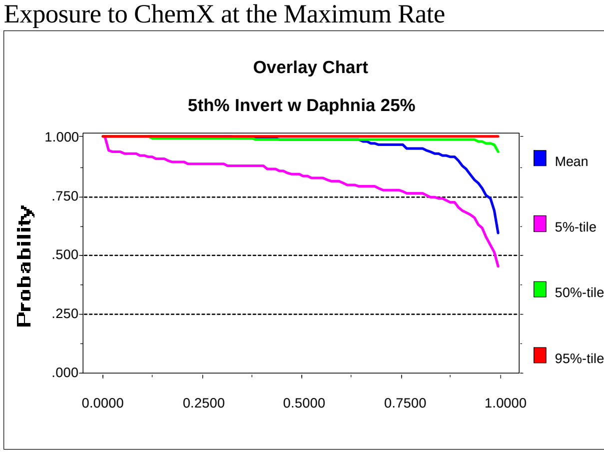


Florida Potatoes: Silversides Mortality Following Peak Exposure to ChemX at the Maximum Rate

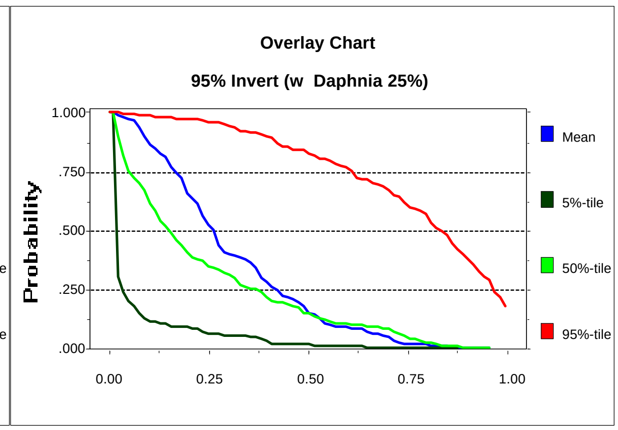
Florida Potatoes: Invertebrates



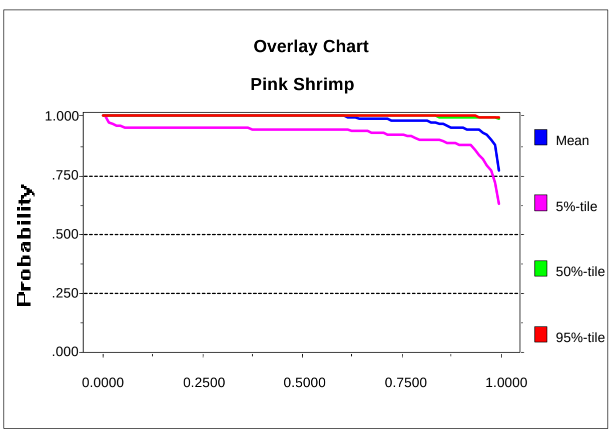
Florida Potatoes: *Daphnia* Mortality Following Peak Exposure to ChemX at the Maximum Rate



Florida Potatoes: 5th% Invertebrate Species Mortality Following Peak Exposure to ChemX at the Maximum Rate

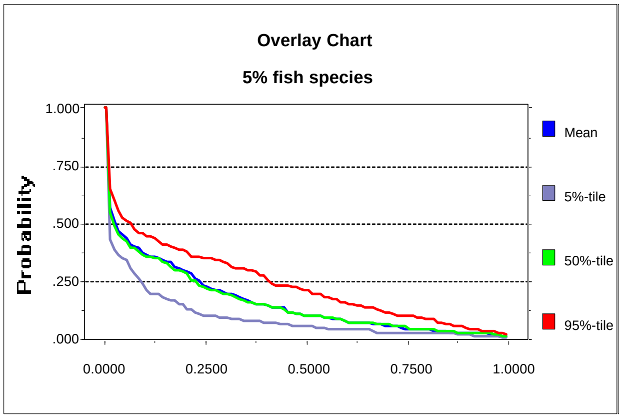


Florida Potatoes: 50th% Invertebrate Species Mortality Following Peak Exposure to ChemX at the Maximum Rate

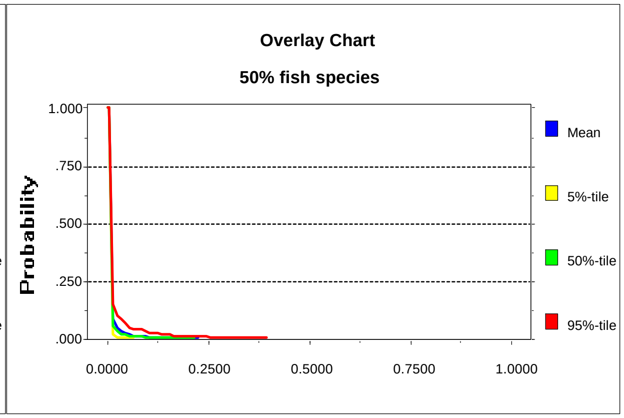


Florida Potatoes: Shrimp Mortality Following Peak Exposure to ChemX at the Maximum Rate

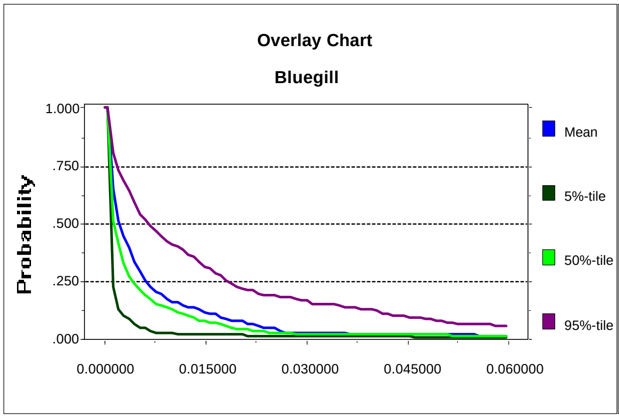
California Grapes: Fish



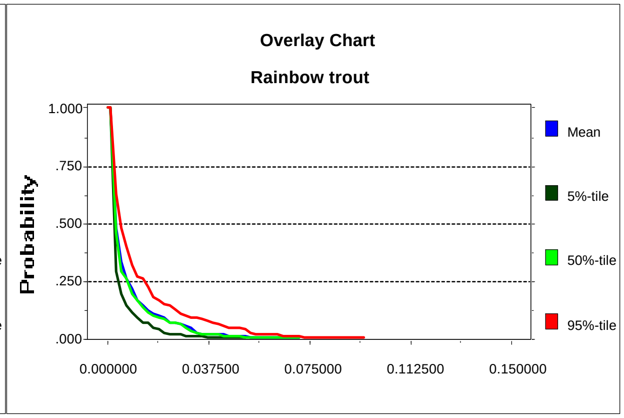
Grapes: 5% Fish Mortality Following Peak Exposure to ChemX at the Maximum Rate



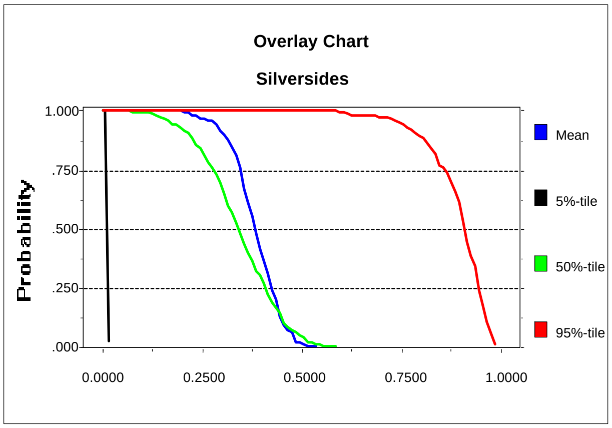
Grapes: 50% Fish Mortality Following Peak Exposure to ChemX at the Maximum Rate



Grapes: Bluegill Mortality Following Peak Exposure to ChemX at the Maximum Rate

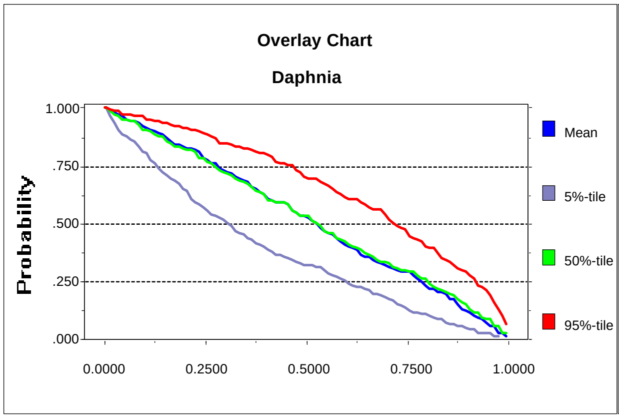


Grapes: Rainbow Trout Mortality Following Peak Exposure to ChemX at the Maximum Rate

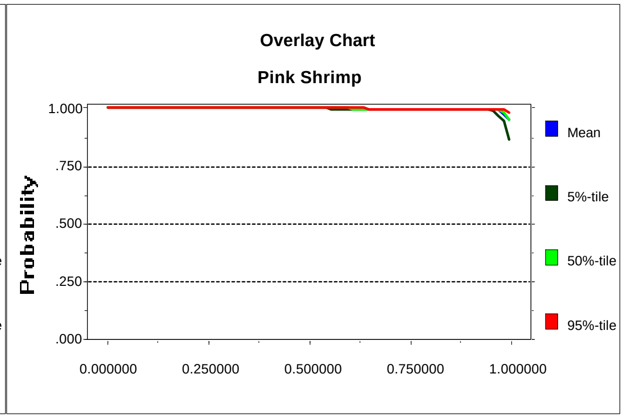


Grapes: Silversides Mortality Following Peak Exposure to ChemX at the Maximum Rate

California Grapes: Invertebrates



Grapes: Daphnia Mortality Following Peak Exposure to ChemX at the Maximum Rate

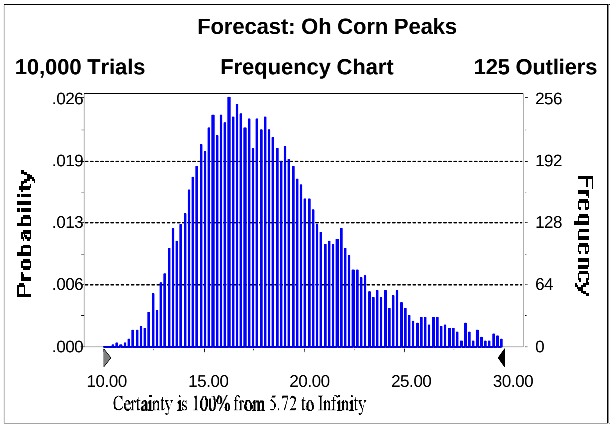


Grapes: Shrimp Mortality Following Peak Exposure to ChemX at the Maximum Rate

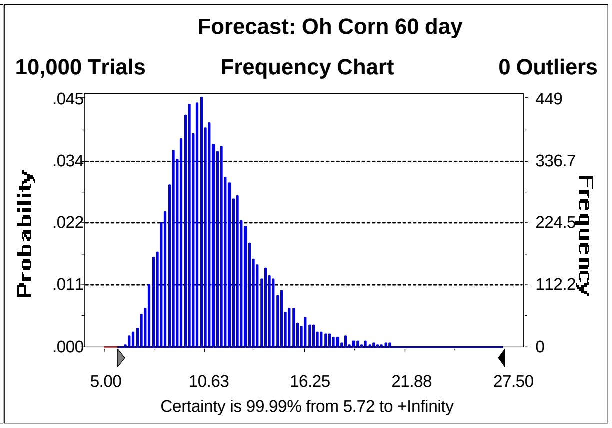
Appendix H: Graphs of Probability of Exceeding Chronic Endpoint

Corn: Maximum Application Rate

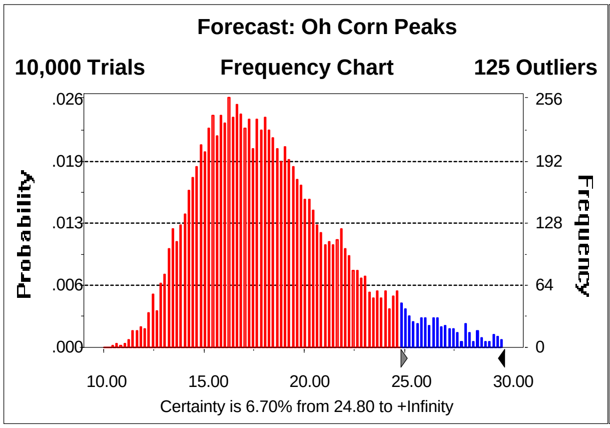
In the exceedence frequency graphs, the blue areas indicate the probability that exposure concentrations will exceed the chronic endpoint. The red indicates probability of not exceeding the chronic endpoint. The certainty of exceeding the chronic endpoint is given on the bottom center of each graph, and the arrows on the x-axis indicate the exposure concentration range for which the endpoint is exceeded. The number of outliers given in the upper right hand corner of the graphs simply indicates the number of points not shown in the graph, and only reflects the Commercial Monte Carlo software display window size; these "outliers" were included in the statistical analysis.



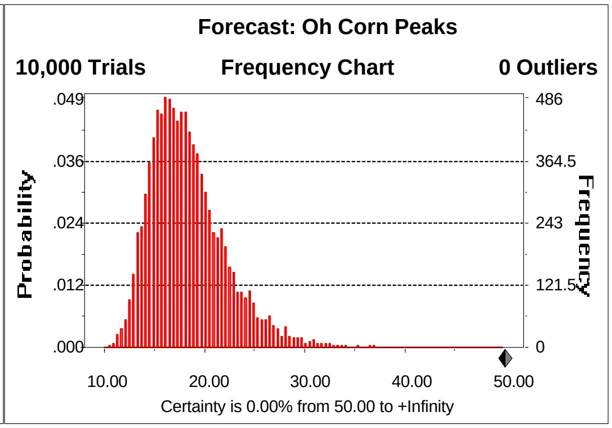
Probability of Exceeding Bluegill ENEC. Annual Peak Concentrations Following Maximum Application of ChemX



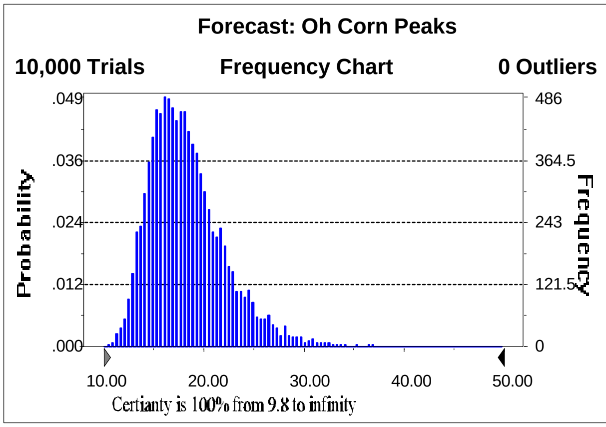
Probability of Exceeding Bluegill ENEC.
Yearly Maxima of 60 Day Average Concentrations Following Maximum Application of ChemX



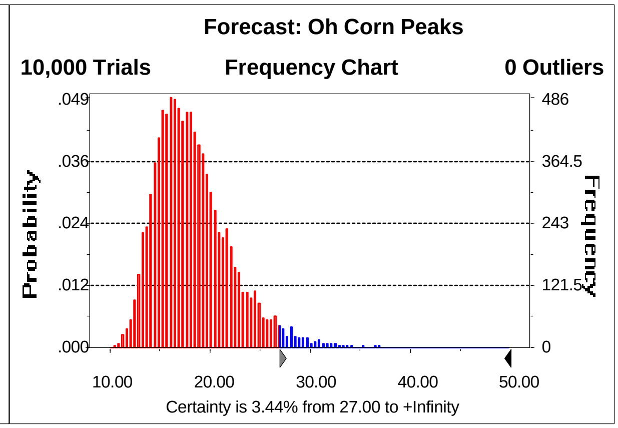
Probability of Exceeding Trout NOEC.
Peak Concentration of ChemX at Maximum Application Rate



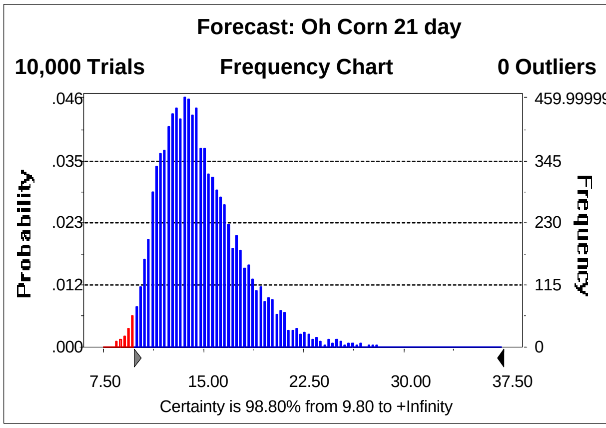
Probability of Exceeding Trout LOEC.
Peak Concentration of ChemX at Maximum Application Rate



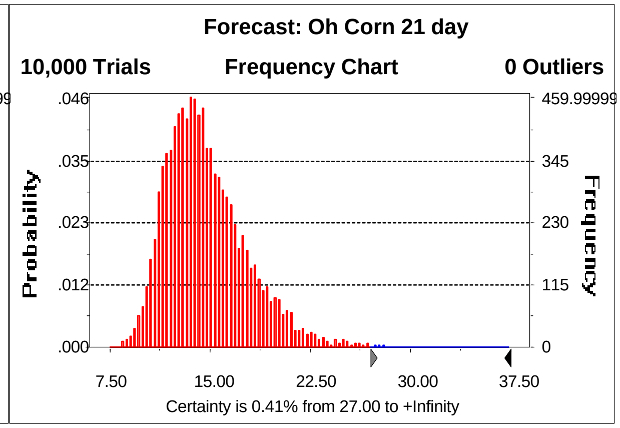
Probability of Exceeding Invertebrate NOEC
Peak Concentration of ChemX at Maximum Application Rate



Probability of Exceeding Invertebrate LOEC. Peak Concentration of ChemX at Maximum Application Rate

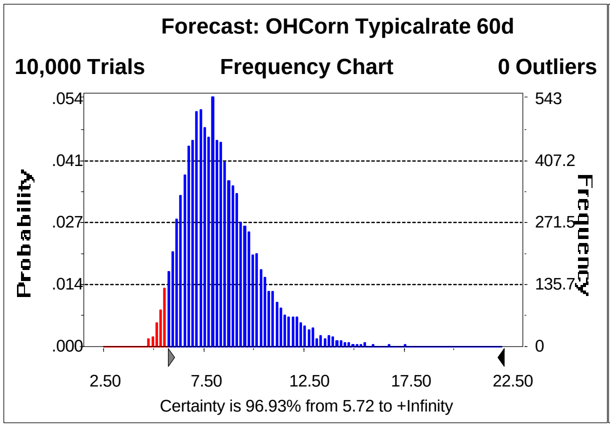


Probability of Exceeding Invertebrate NOEC .
21 day Average Concentration of ChemX at Maximum Application Rate

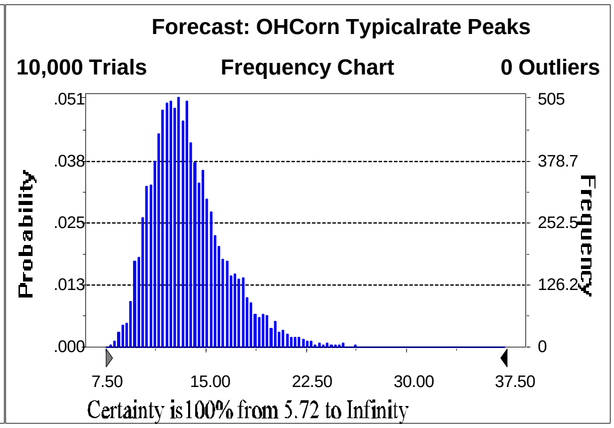


Probability of Exceeding Invertebrate LOEC. 21 Day Average Concentration of ChemX at Maximum Application Rate

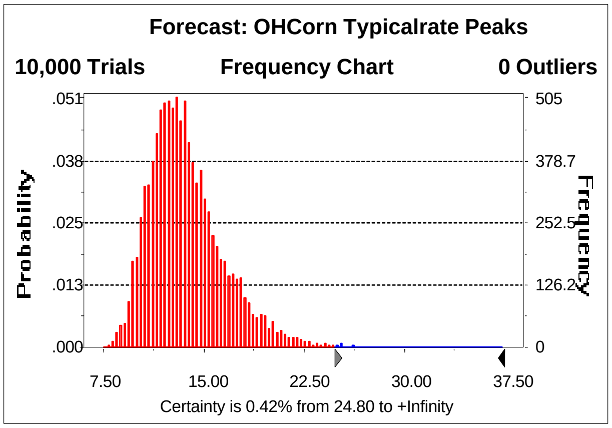
Corn: Typical Application Rate



Probability of Exceeding Bluegill ENEC.
60 Day Average Concentration of ChemX at Typical Application Rate

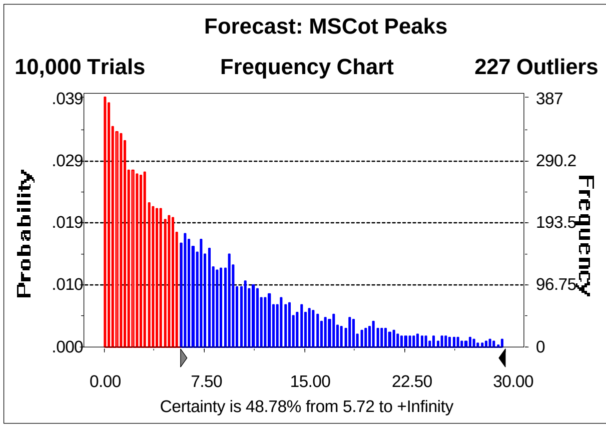


Probability of Exceeding Bluegill ENEC.Peak Concentration of ChemX at Typical Application Rate

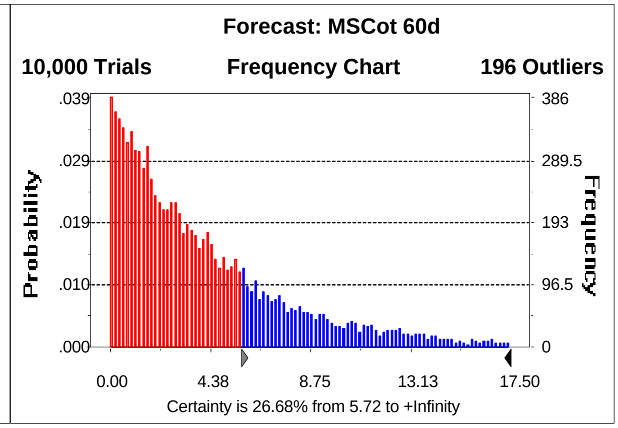


Probability of Exceeding Trout NOEC.
Peak Concentration of ChemX Following Application on Corn at the Typical Rate

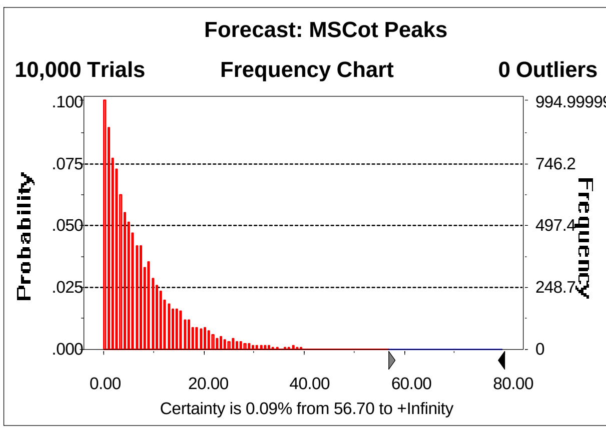
Mississippi Cotton



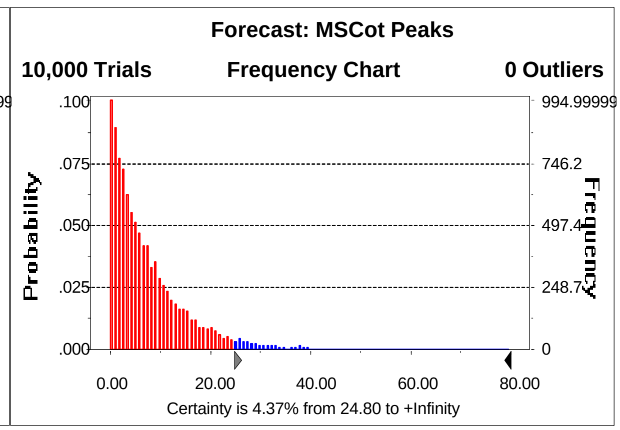
Probability of Exceeding Bluegill ENEC.
Peak Concentration of ChemX at Maximum Application Rate



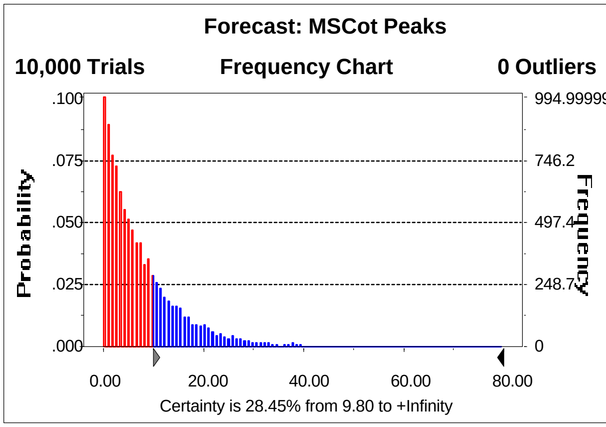
Probability of Exceeding Bluegill ENEC.
60 Day Average Concentration of ChemX at Maximum Application Rate



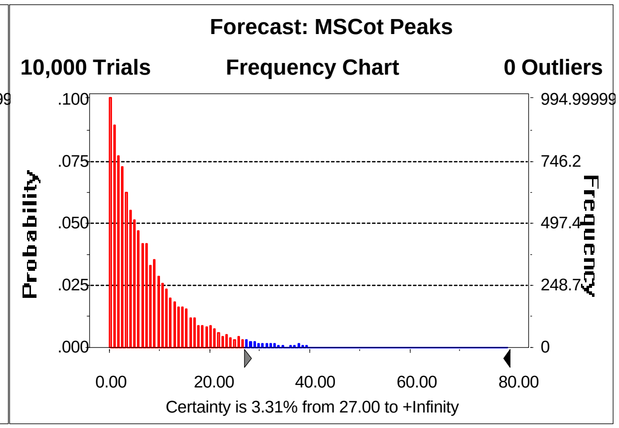
Probability of Exceeding Trout LOEC.
Peak Concentration of ChemX at Maximum Application Rate



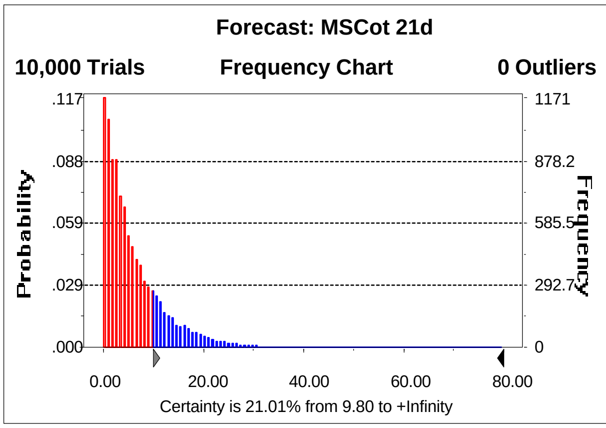
Probability of Exceeding Trout NOEC.
Peak Concentration of ChemX at Maximum Application Rate



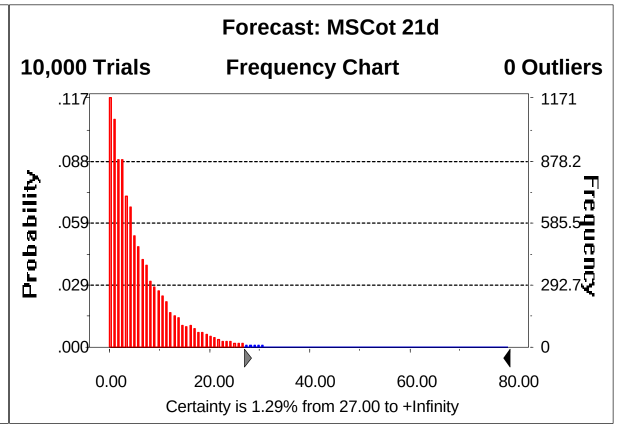
Probability of Exceeding Invertebrate NOEC.
Peak Concentration of ChemX at Maximum Application Rate



Probability of Exceeding Invertebrate LOEC.
Peak Concentration of ChemX at Maximum Application Rate

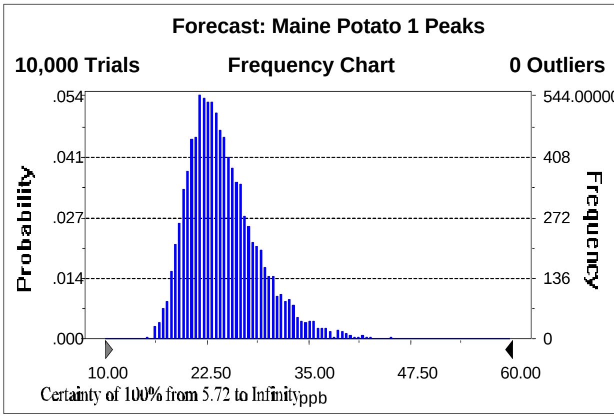


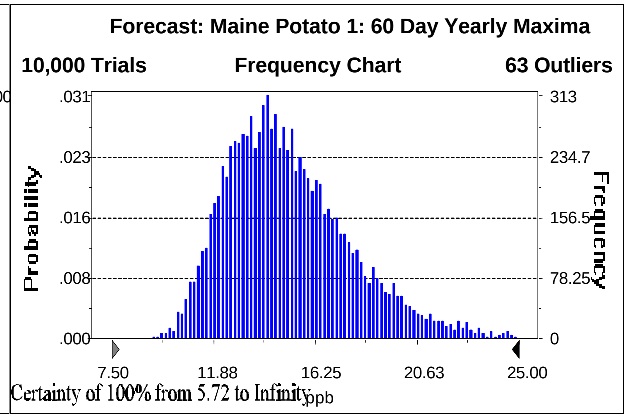
Probability of Exceeding Invertebrate NOEC.
21 Day Average Concentration at Maximum Application Rate



Probability of Exceeding Invertebrate LOEC.
21 day Average Concentration at Maximum Application Rate

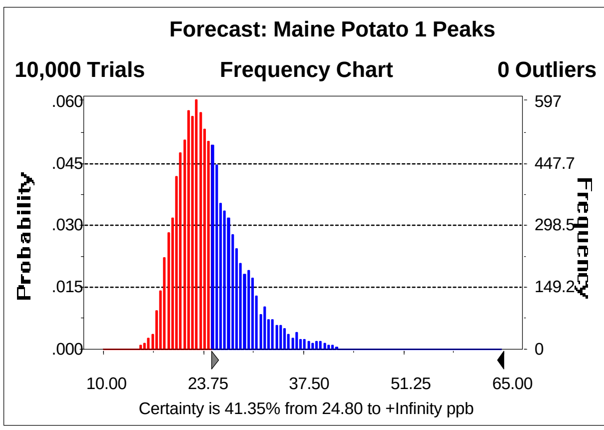
Potatoes: Maximum Application Rate

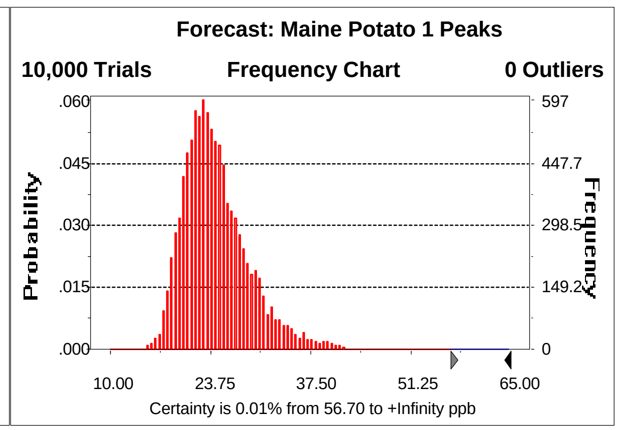




Probability of Exceeding Bluegill ENEC.
Peak Concentration of ChemX at Maximum Rate

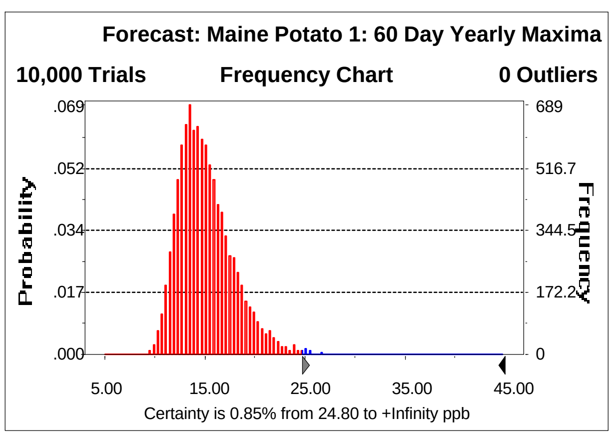
Probability of Exceeding Bluegill ENEC. 60-Day
Average Concentration at Maximum Rate



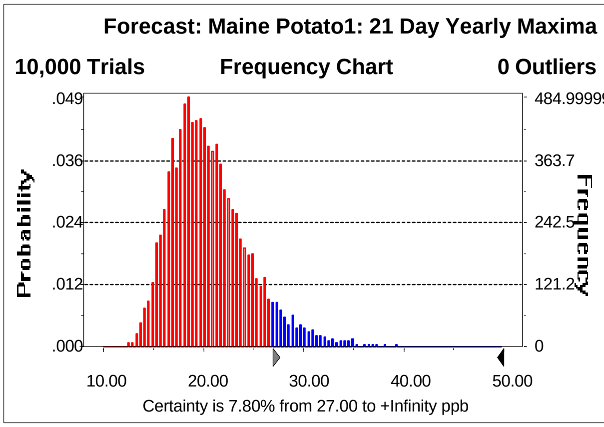


Probability of Exceeding Trout NOEC.
Peak Concentration of ChemX at Maximum Rate

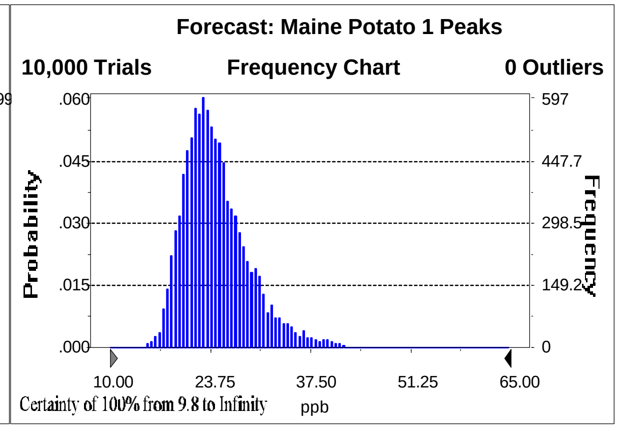
Probability of Exceeding Trout LOEC.
Peak Concentration of ChemX at Maximum Rate



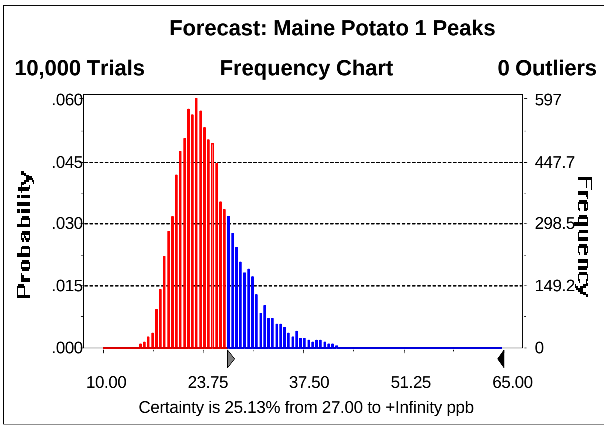
Probability of Exceeding trout NOEC.
60 day Average Concentration of ChemX at Maximum
Rate



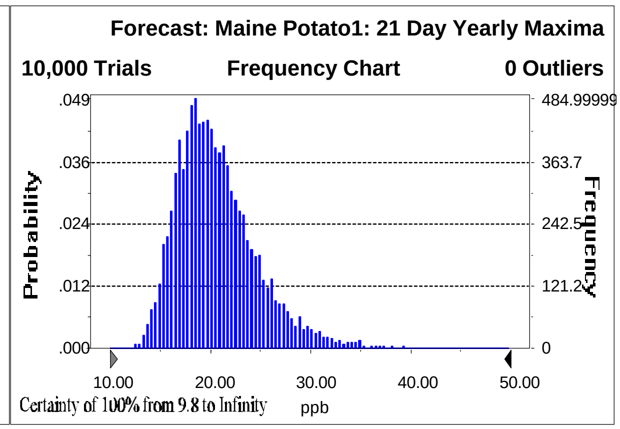
Probability of Exceeding Invertebrate LOEC.
21 Day Average Concentration of ChemX at Maximum Rate



Probability of Exceeding Invertebrate NOEC.
Peak Concentration of ChemX at Maximum Rate

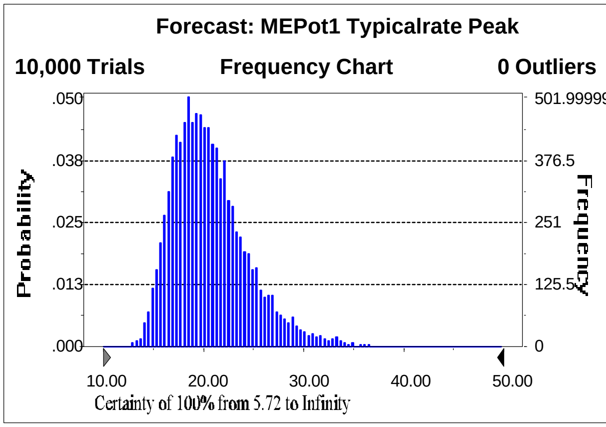


Probability of Exceeding Invertebrate LOEC.
Peak Concentration of ChemX at Maximum Rate

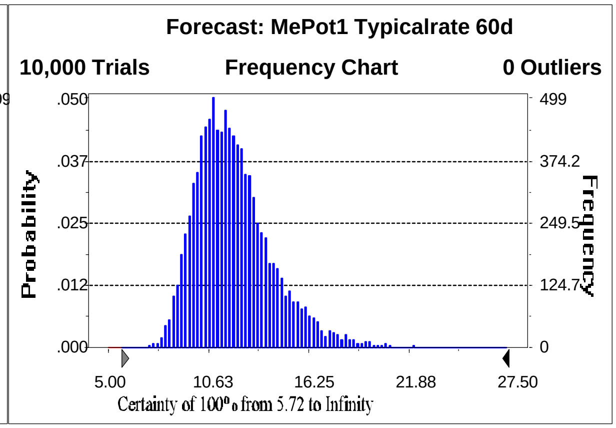


Probability of Exceeding Invertebrate NOEC.
21 Day Average Concentration of ChemX at Maximum Rate

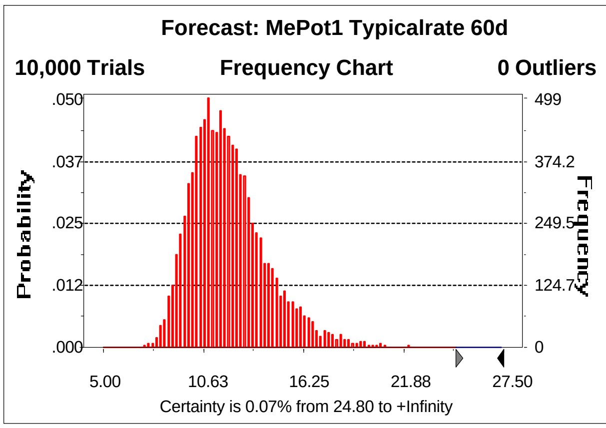
Potatoes: Average Application Rate



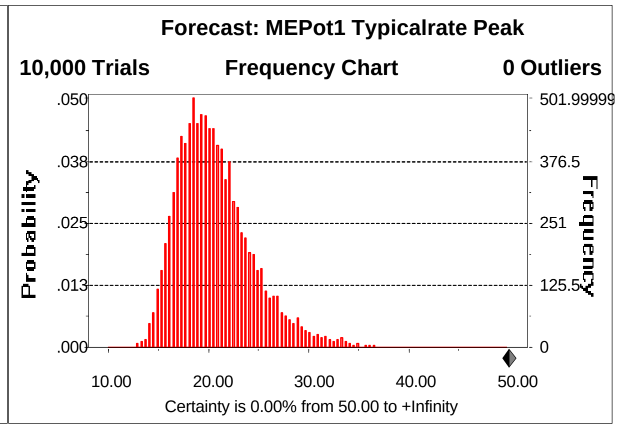
Probability of Exceeding Bluegill ENEC.
Peak Concentration of ChemX at Average Rate



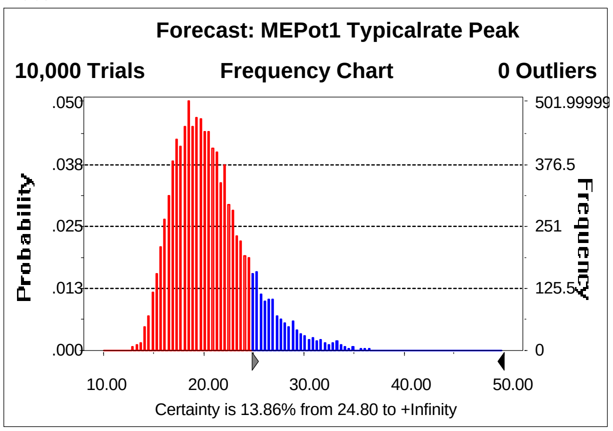
Probability of Exceeding Bluegill ENEC.
60 Day Average Concentration of ChemX at Average Rate



Probability of Exceeding Trout NOEC
60 Day Average Concentration of ChemX at Average Rate

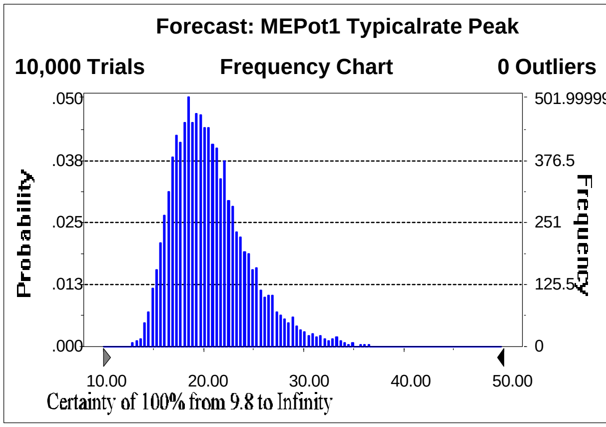


Probability of Exceeding Trout LOEC
Peak Concentration of ChemX at Average Rate

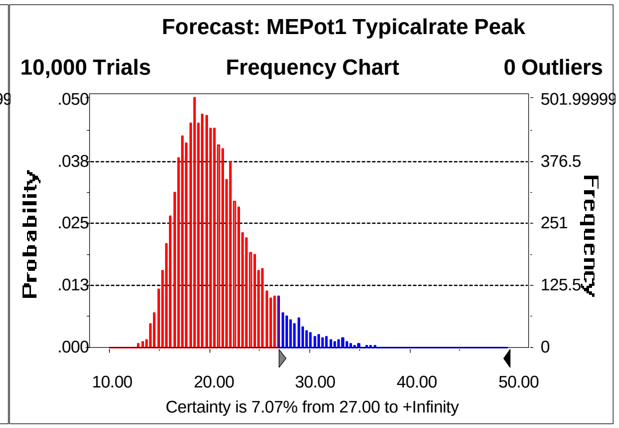


Probability of Exceeding Trout NOEC.
Peak Concentration of ChemX at Average Rate

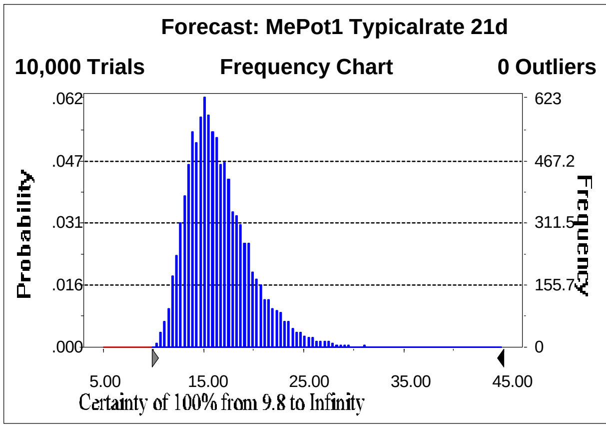
Maine Potatoes Typical Rate



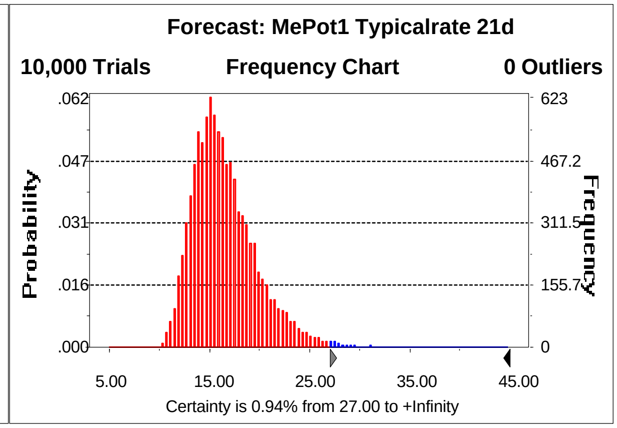
Probability of Exceeding Invertebrate NOEC.
Peak Concentration of ChemX at Average Application Rate



Probability of Exceeding Invertebrate LOEC.
Peak Concentration of ChemX at Average Application Rate

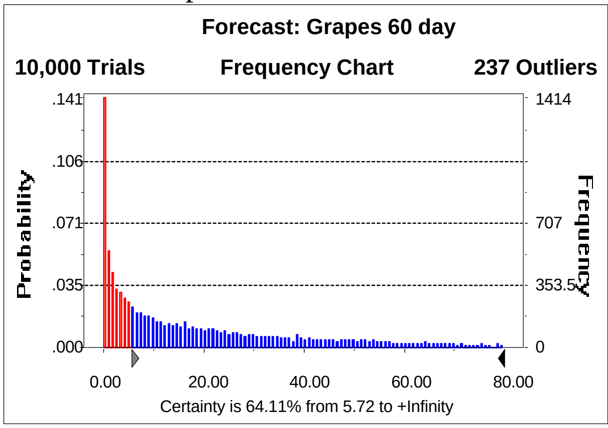


Probability of Exceeding Invertebrate NOEC.
21 Day Average Concentration of ChemX at Average Application Rate

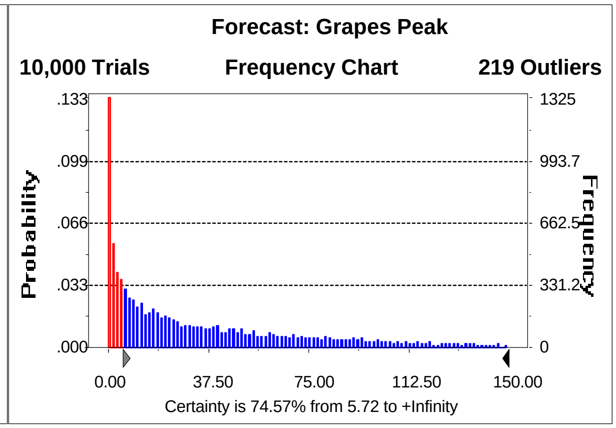


Probability of Exceeding Invertebrate LOEC.
21 Day Average Concentration at Average Application Rate

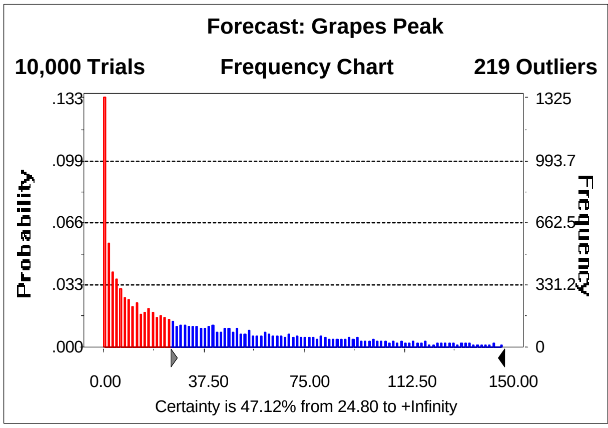
California Grapes- Maximum Rate



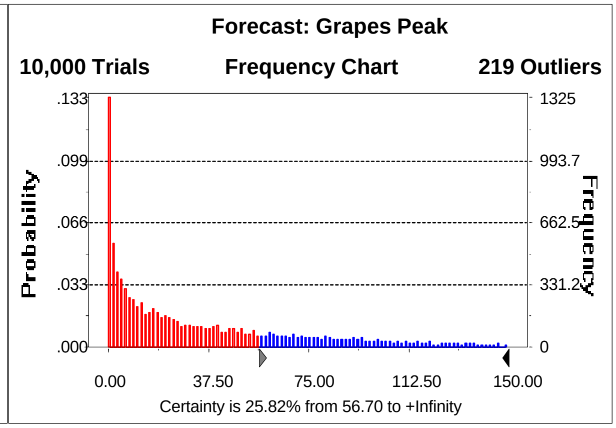
Probability of Exceeding Bluegill ENEC.
60 Day Average Concentration at Maximum Rate



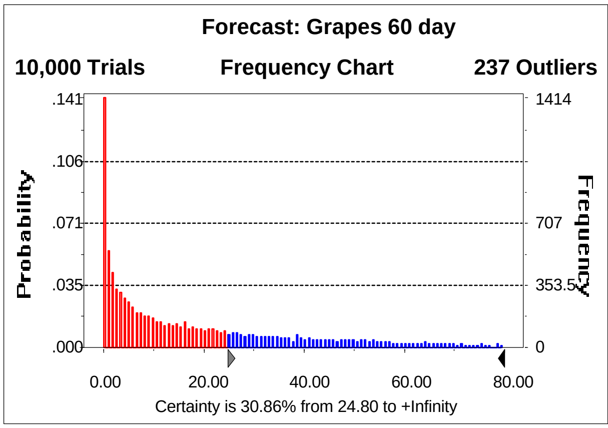
Probability of Exceeding Bluegill ENEC.
Peak Concentration at Maximum Rate



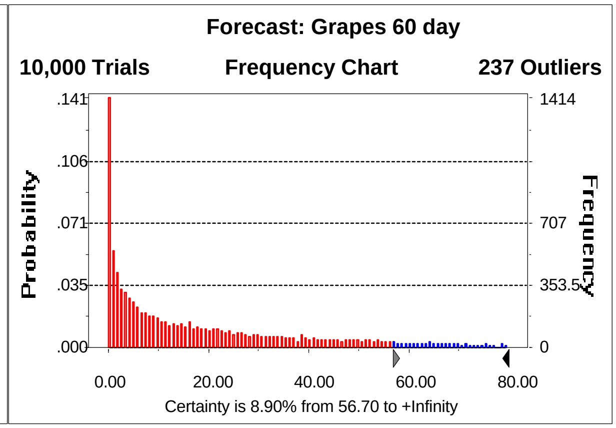
Probability of Exceeding Trout NOEC.
Peak Exposure to ChemX at Maximum Rate



Probability of Exceeding Trout LOEC.
Peak Exposure to ChemX at Maximum Rate

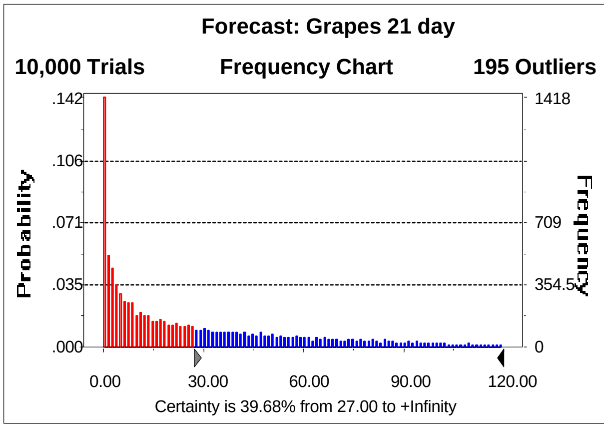


Probability of Exceeding Trout NOEC.
60 Day Average Concentration of ChemX at Maximum Rate

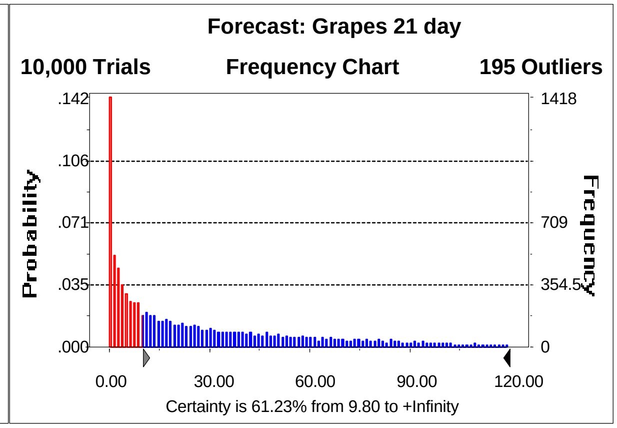


Probability of Exceeding Trout LOEC.
60 Day Average Concentration of ChemX at Maximum Rate

California Grapes - Maximum Rate

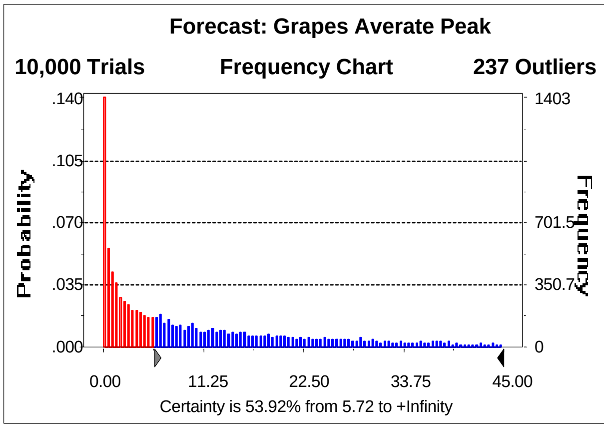


Probability of Exceeding Invertebrate LOEC.
21 day Average Concentration of ChemX at Maximum Rate

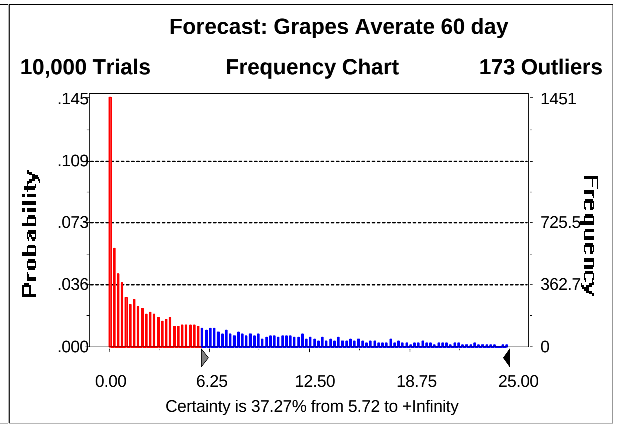


Probability of Exceeding Invertebrate NOEC.
21 day Average Concentration of ChemX at Maximum Rate

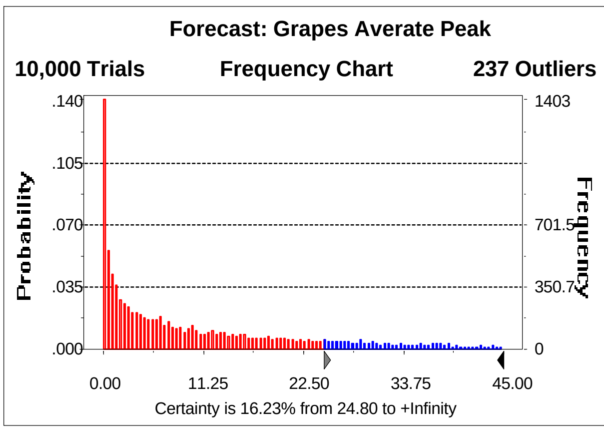
California Grapes - Average Rate



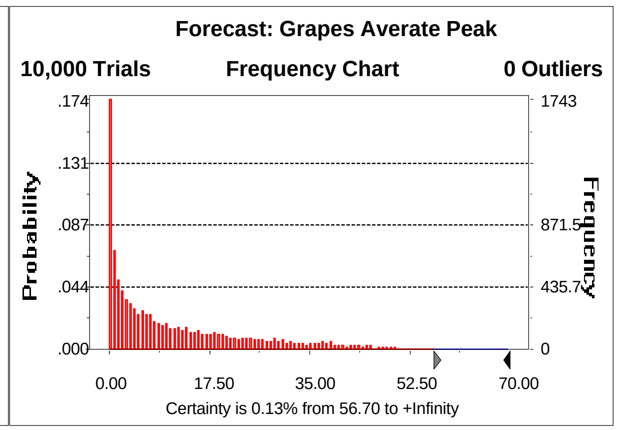
Probability of Exceeding Bluegill ENEC.
Peak Concentration



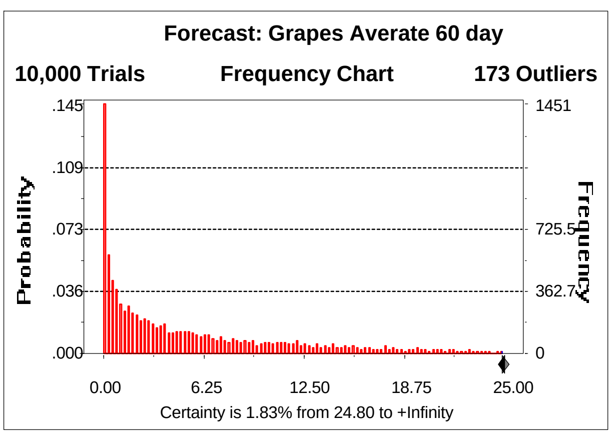
Probability of Exceeding Bluegill ENEC.
60 day Average Concentration of ChemX at Average Application Rate



Probability of Exceeding Trout NOEC.
Peak Concentration of ChemX at Average Application Rate

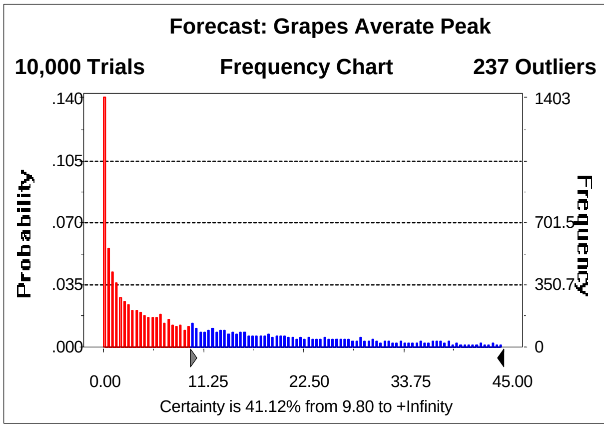


Probability of Exceeding Trout LOEC.
Peak Concentration of ChemX at Average Application Rate

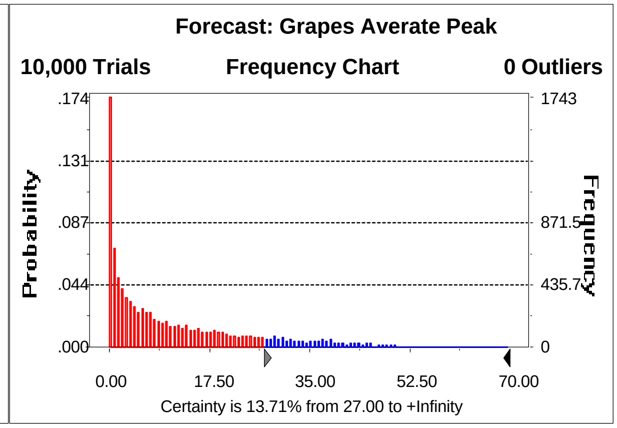


Probability of Exceeding Trout NOEC.
60 Day Average Concentration at Average Rate

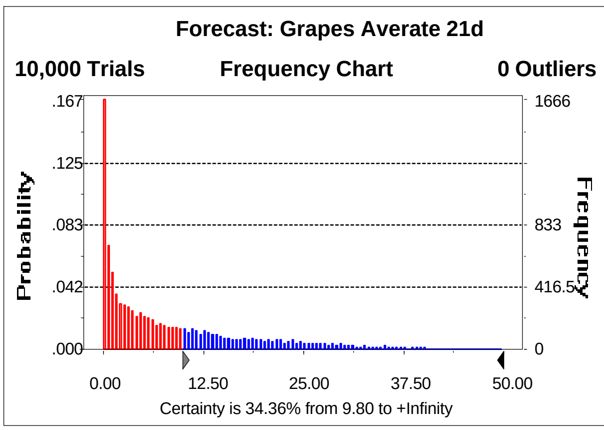
California Grapes- Average Rate



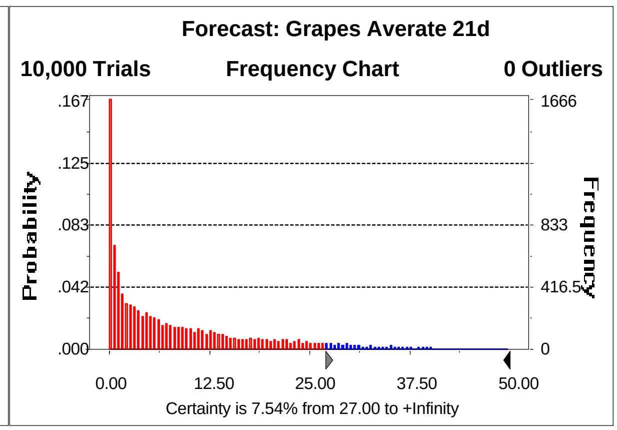
Probability of Exceeding Invertebrate NOEC.
Peak Concentration of ChemX at Average Application Rate



Probability of Exceeding Invertebrate LOEC.
Peak Concentration of ChemX at Average Application Rate



Probability of Exceeding Invertebrate NOEC.
21 day Average Concentration of ChemX at Average Rate



Probability of Exceeding Invertebrate LOEC.
21 Day Average Concentration of ChemX at Average Application Rate